STIC Search Report
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TO: Rei-Tsang Shiao **Location: 5a10 / 5c18** **Wednesday, October 13, 2004** **Art Unit: 1626** **Phone: 272-0707** **Serial Number: 10 / 650020**	**From: Jan Delaval** **Location: Biotech-Chem Library** **Rem 1A51** **Phone: 272-2504** **jan.delaval@uspto.gov**

Search Notes

Jan Delcroix for search

Access DB# 134528

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Robert (Kathy) Shiao Examiner #: 79521 Date: 10/6/04

Art Unit: 1626 Phone Number 30 2-0707 Serial Number: 10/650,020

Mail Box and Bldg/Room Location: 5A10/5C18 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need. ME

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

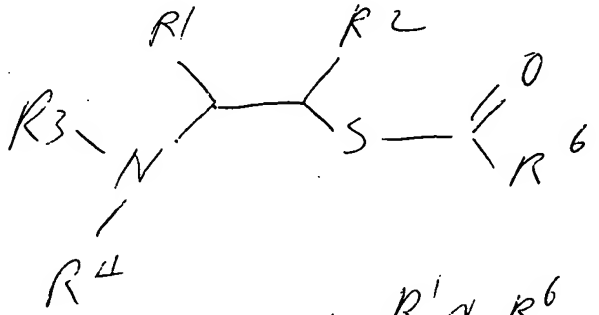
Title of Invention: Taylor amd cpd

Inventors (please provide full names): Yang et al

Earliest Priority Filing Date: _____

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

1. Search a compd of formula (I)



1. R1 & R6 are sub

2 R3, R4 and N form a hetrocycle, a hetaryl ring (3-8 ring)

****

STAFF USE ONLY

Searcher: am

Searcher Phone #: 22504

Searcher Location: _____

Date Searcher Picked Up: 10/13

Date Completed: 10/13

Searcher Prep & Review Time: _____

Clerical Prep Time: K

Online Time: ~ 20

Type of Search

NA Sequence (#) _____

AA Sequence (#) _____

Structure (#) ✓

Bibliographic _____

Litigation _____

Fulltext _____

Patent Family _____

Other _____

Vendors and cost where applicable

STN ✓

Dialog _____

Questel/Orbit _____

Dr.Link _____

Lexis/Nexis _____

Sequence Systems _____

WWW/Internet _____

Other (specify) _____

PTO-1590 (8-01)

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STRUCTURE FILE UPDATES:   12 OCT 2004  HIGHEST RN 761381-83-3
DICTIONARY FILE UPDATES:  12 OCT 2004  HIGHEST RN 761381-83-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
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http://www.cas.org/ONLINE/DBSS/registryss.html

=> d sta que l21
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                 571148-37-3/BI OR 100-52-7/BI OR 111-24-0/BI OR 111061-16-6/BI
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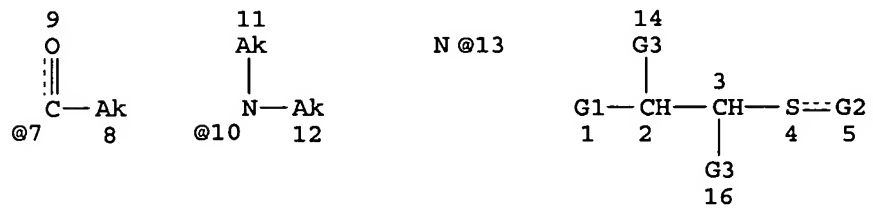


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VAR G1=10/13
VAR G2=CHO/7
VAR G3=AK/CY
NODE ATTRIBUTES:
NSPEC   IS R      AT  13
CONNECT IS M1  RC AT  13
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  14
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STEREO ATTRIBUTES: NONE
L15          25 SEA FILE=REGISTRY CSS FUL L13
L16          10 SEA FILE=REGISTRY ABB=ON  PLU=ON  L11 AND L15
L18          15 SEA FILE=REGISTRY ABB=ON  PLU=ON  L15 NOT L16
L19          13 SEA FILE=REGISTRY ABB=ON  PLU=ON  L18 NOT (C19H21NOS OR
                C25H25NOS)
L21          23 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L16 OR L19)


=> d his

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                SET COST OFF

     FILE 'HCAPLUS' ENTERED AT 15:13:55 ON 13 OCT 2004
L1            2 S (US2002-039557# OR US2003-650020#)/AP,PRN
                E YANG T/AU
L2          187 S E3,E20,E21
                E YANG TENG/AU
L3           49 S E3,E10
L4            3 S E13
                E CHEN N/AU
L5           99 S E3,E14
                E CHEN NAN/AU
L6          131 S E3,E15
                E LIU T/AU
L7          822 S E3-E37
                E LIU TO/AU
L8            2 S E3
L9          483 S LIU TO?/AU
L10           2 S L1 AND L2-L9
                SEL RN

     FILE 'REGISTRY' ENTERED AT 15:17:09 ON 13 OCT 2004
L11          53 S E1-E53
L12          11 S L11 AND (N AND S AND O)/ELS
L13             STR
L14           1 S L13 CSS SAM
L15          25 S L13 CSS FUL
                SAV L15 SHIAO650/A
L16          10 S L11 AND L15
L17           1 S L12 NOT L16
L18          15 S L15 NOT L16
L19          13 S L18 NOT (C19H21NOS OR C25H25NOS)
L20           2 S L18 NOT L19
L21          23 S L16,L19

     FILE 'HCAOLD' ENTERED AT 15:22:44 ON 13 OCT 2004
L22           3 S L21
                SEL AN
                EDIT E54-E56 /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 15:23:10 ON 13 OCT 2004
L23           5 S E54-E56

     FILE 'HCAOLD' ENTERED AT 15:23:42 ON 13 OCT 2004

     FILE 'HCAPLUS' ENTERED AT 15:24:43 ON 13 OCT 2004
L24           4 S L23 NOT ASINGER ?/AU
L25          12 S L21
L26           2 S L25 AND L1-L10
L27          14 S L24-L26
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                E ADDITION REACTION/CT
L28           8 S L27 AND (E3+OLD,NT,PFT,RT OR E46+OLD,NT,PFT,RT OR E58+OLD,NT,
L29           7 S L27 AND (ALDEHYDE OR KETONE)
L30           0 S L27 AND CARBONYL
L31           4 S L27 AND LIGAND

     FILE 'REGISTRY' ENTERED AT 15:27:43 ON 13 OCT 2004
L32           3 S (ZINC OR COPPER OR TITANIUM)/CN

     FILE 'HCAPLUS' ENTERED AT 15:28:04 ON 13 OCT 2004
L33           1 S L27 AND L32
L34           4 S L27 AND (ZN OR ZINC OR CU OR COPPER OR TI OR TITAN?)
L35           0 S L27 AND ?METAL?(L)?COMPLEX?
L36          14 S L27-L31,L33-L35
L37          14 S L36 AND (PD<=20020108 OR PRD<=20020108 OR AD<=20020108)
L38           2 S L37 AND ORGANOMETAL?/SC,SX
L39          12 S L37 NOT L38
L40           4 S L39 AND L24
L41           8 S L39 NOT L40

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=> fil hcaold
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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate
substance identification.  Title keywords, authors, patent
assignees, and patent information, e.g., patent numbers, are
now searchable from 1907-1966.  TIFF images of CA abstracts
printed between 1907-1966 are available in the PAGE
display formats.

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all substance data from the REGISTRY file.  Enter HELP FIRST for
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=> d all hitstr tot l22

L22  ANSWER 1 OF 3  HCAOLD  COPYRIGHT 2004 ACS on STN
AN   CA62:1588c  CAOLD
TI   phenylmercaptoalkylamines - (IV) configurations of N-alkyl-1-phenyl-2-
     chloropropylamines and their rearrangements with nucleophilic reagents,
     (V) rearrangements of 1-phenyl-2-chloroethylamines with nucleophilic
     reagents
AU   Nishimura, Haruki; Takamatsu, H.
IT    934-12-3    934-14-5    934-15-6    936-42-5    936-43-6    938-89-6
     938-90-9    939-41-3    939-42-4    939-43-5    939-44-6    939-45-7
     939-46-8    939-47-9    942-47-2    942-61-0    945-44-8    945-55-1
     945-67-5    951-62-2    952-18-1    952-19-2    980-86-9   1008-64-6
     1009-10-5   1011-31-0   1011-32-1   1014-13-7   1017-00-1   1017-01-2
     1076-52-4   1081-29-4   1084-48-6   1128-33-2   1131-50-6   1140-76-7
     1165-97-5   1201-46-3   1201-56-5   1210-30-6   1246-84-0
     1444-33-3   1630-39-3   1630-40-6   1797-76-8   2202-60-0   2202-61-1
     2202-62-2   2202-63-3   2202-64-4   2202-65-5   2202-66-6   2202-67-7
     2202-68-8   2202-69-9   2202-70-2   2202-71-3   2218-01-1   2218-08-8
     2226-26-8   2226-27-9   2226-28-0   2226-29-1   2226-30-4   2226-31-5
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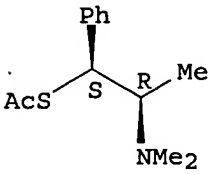
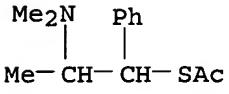
2226-32-6 2226-33-7 2226-34-8 2226-35-9 3373-07-7 3852-66-2
4561-45-9 6721-66-0 6853-14-1 20245-69-6 22083-26-7 62278-80-2
67428-86-8 67921-36-2 68277-68-9 68277-71-4 86117-29-5 90944-85-7
90944-86-8 91341-40-1 91428-40-9 91428-41-0 91553-45-6 91553-46-7
91553-52-5 **92196-51-5** 92286-72-1 92644-98-9 93018-37-2
93653-73-7 94264-26-3 94520-92-0 95697-03-3 96675-54-6 97044-99-0

IT **1210-30-6 92196-51-5**
RN 1210-30-6 HCAOLD
CN Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester, erythro- (8CI) (CA INDEX NAME)

Relative stereochemistry.



RN 92196-51-5 HCAOLD
CN Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester (7CI) (CA INDEX NAME)



L22 ANSWER 2 OF 3 HCAOLD COPYRIGHT 2004 ACS on STN
AN CA62:1587g CAOLD
TI phenylmercaptoalkylamines - (II) configuration of 1-phenyl-2-alkylaminopropane-thiol, (III) Hofman degradation of 1-phenyl-2-dimethylaminopropanethiol quaternary salt
AU Nishimura, Haruki
IT 645-62-5 934-14-5 934-45-2 942-45-0 942-48-3 942-49-4
942-50-7 942-94-9 944-90-1 952-49-8 952-52-3 953-35-5
985-30-8 985-55-7 985-81-9 986-81-2 988-62-5 988-67-0
1006-92-4 1009-10-5 1009-16-1 1011-25-2 1011-63-8 1011-64-9
1014-35-3 1017-25-0 1017-26-1 1020-12-8 1022-11-3 1052-18-2
1078-37-1 1079-60-3 1081-29-4 1083-08-5 1083-13-2 1083-24-5
1084-49-7 1094-73-1 1094-81-1 1099-08-7 1102-17-6 1103-56-6
1104-61-6 1105-90-4 1111-14-4 1131-81-3 1201-81-6 1245-54-1
1262-51-7 1444-32-2 1498-99-3 1630-36-0 1667-57-8 2202-56-4
2202-57-5 2202-58-6 2202-59-7 2218-05-5 2218-07-7 2218-08-8
2218-09-9 2218-10-2 2218-11-3 2218-12-4 2218-13-5 2218-14-6
2218-15-7 2218-16-8 2218-17-9 2218-18-0 2218-19-1 2218-20-4
2218-21-5 2218-22-6 2218-23-7 2218-24-8 2218-25-9 2226-20-2
2226-21-3 **2226-22-4** **2226-23-5** 2226-25-7
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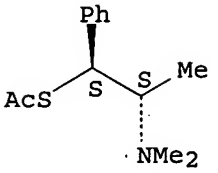
91248-86-1 91341-40-1 91341-41-2 91428-45-4 **92196-51-5**
92286-72-1 93002-42-7 93650-92-1 94489-15-3 94756-09-9 94960-76-6
95845-16-2 95954-09-9 96279-67-3 97044-99-0 97828-11-0 101379-38-8
104695-69-4

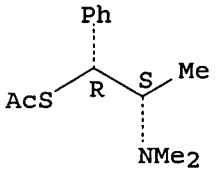
IT **2226-22-4 2226-23-5 92196-51-5**
RN 2226-22-4 HCAOLD
CN Ethanethioic acid, S-[2-(dimethylamino)-1-phenylpropyl] ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

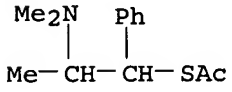


RN 2226-23-5 HCAOLD
CN Ethanethioic acid, S-[2-(dimethylamino)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

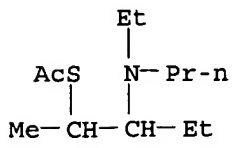
Absolute stereochemistry.



RN 92196-51-5 HCAOLD
CN Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester (7CI) (CA INDEX NAME)



L22 ANSWER 3 OF 3 HCAOLD COPYRIGHT 2004 ACS on STN
AN CA55:2616e CAOLD
TI concomitant reaction of elemental S and gaseous NH3 on ketones - (XXIV) thiazolidines and thiazoles from α-mercapto ketones
AU Asinger, Friedrich; Thiel, M.; Hauthal, H. G.
TI cyclization of N-allylthioamides and their homologs with particular attention to thiazoline synthesis
AU Sullivan, John M.
IT 32272-57-4 52414-89-8 52414-91-2 86290-19-9 87116-68-5 91560-78-0 98428-86-5 98487-47-9 98545-06-3 98957-53-0 98958-47-5 98998-96-0 99863-95-3 99863-96-4 99868-79-8 100248-09-7 **100387-18-6** 100450-79-1 100523-64-6 100529-74-6 100705-03-1 100799-45-9 100887-65-8 100967-63-3 101088-18-0 101088-19-1 101271-03-8 101440-49-7 102020-10-0 102161-40-0 106522-28-5 107682-90-6 108955-57-3
IT **100387-18-6**
RN 100387-18-6 HCAOLD
CN 2-Pentanethiol, 3-(ethylpropylamino)-, acetate (ester) (6CI) (CA INDEX NAME)



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FILE COVERS 1907 - 13 Oct 2004  VOL 141 ISS 16
FILE LAST UPDATED: 12 Oct 2004  (20041012/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> d all hitstr tot l40

L40  ANSWER 1 OF 4  HCAPLUS  COPYRIGHT 2004 ACS on STN
AN   1965:8905  HCAPLUS
DN   62:8905
OREF 62:1588c-e
ED   Entered STN:  22 Apr 2001
TI   Phenylmercaptoalkylamines. IV. Configurations of N-alkyl-1-phenyl-2-
     chloropropylamines and their rearrangements with nucleophilic reagents
AU   Nishimura, Haruki; Takamatsu, Hideji
CS   Dainippon Pharm. Co., Ltd., Osaka, Japan
SO   Yakugaku Zasshi (1964), 84(9), 817-24
     CODEN: YKKZAJ; ISSN: 0031-6903
DT   Journal
LA   Japanese
CC   35 (Noncondensed Aromatic Compounds)
AB   Treatment of DL-erythro-1-methylamino-1-phenyl-2-propanol (I) with SOCl2
     gives erythro-N-methyl-1-phenyl-2-chloropropylamine-HCl (II), m.
     210° (decomposition), while treatment of I with PCl5 gives the
     corresponding threo compound (IIa), m. 150-3°.  Na2S2O3 and II and
     IIa gives erythro-1-phenyl-2-methylaminopropylthiosulfonic acid (III) [m.
     239° (decomposition)] and the corresponding threo compound (IIIa) [m.
     199-200° (decomposition)], resp.  This reaction proceeds with two Walden
     inversions via the intermediate aziridinium compound  Treatment of II and
     IIa with NaOH affords DL-threo-3-phenyl-1,2-dimethylaziridine (picrate m.
     142-4°) and the corresponding erythro compound (picrate m.
     97.5-8.5°), resp.  Also is prepared erythro-N,N-dimethyl-1-phenyl-2-
     chloropropylamine-HCl (m. 169-70°) by chlorination of
     erythro-1-dimethylamino-1-phenyl-2-propanol-HCl with PCl5; no threo-type
     Cl derivative is obtained.
IT   Nuclear magnetic resonance
     Stereochemistry
        (of (1,2-epithiopropyl)benzenes and (1,2-epoxypropyl)benzenes)
IT   Stereochemistry
        (of α-(1-chloroethyl)benzylamine N-alkyl derivs.)
IT   Rearrangements
        (of α-(1-chloroethyl)benzylamine N-alkyl derivs. by nucleophiles)
```

IT Nucleophiles
(reaction with N-alkyl-α-(1-chloroethyl)benzylamines)
IT Acetamide, N,N'-[dithiobis(1-methyl-2-phenylethylene)]bis[N-methyl-, L(-)-erythro-
Acetamide, N-(β-mercapto-α-methylphenethyl)-N-methyl-, acetate, L-(-)-erythro-
Acetic acid, thio-, S-esters with (β-mercapto-α-methylphenethyl)trimethylammonium iodide, erythro-
Acetic acid, thio-, S-esters with N-(β-mercapto-α-methylphenethyl)-N-methylacetamide, L-(-)-erythro-
Benzyl alcohol, α-[(dimethylamino)methyl]-, hydrochloride, D(-)-, DL-
Benzyl alcohol, α-[(dimethylamino)methyl]-, hydrochloride, L(+)-
Benzylamine, α-(1-chloroethyl)-N-methyl-, hydrochloride, three-
Benzylamine, α-(1-chloroethyl)-N-methyl-, hydrochloride, three-
Phenethyl alcohol, β-(dimethylamino)-, hydrochloride, DL-
Phenethyl alcohol, β-(dimethylamino)-, D-(-)-
Phenethyl alcohol, β-(dimethylamino)-, DL-
Phenethylamine, β-ethoxy-N,N-dimethyl-, DL-
Phenethylamine, β-ethoxy-N,N-dimethyl-, L(+)-
Phenethylamine, β-methoxy-N,N,α-trimethyl-, picrate, L(-)-erythro-
Phenethylamine, β-methoxy-N,N,α-trimethyl-, L(-)-erythro-
Pseudourea, 2-[α-[(dimethylamino)methyl]benzyl]-2-thio-, dihydrochloride, D(-)-
Pseudourea, 2-[α-[(dimethylamino)methyl]benzyl]-2-thio-, dihydrochloride, L(+)-
Thiosulfuric acid, H2S2O3, S-[α-(aminomethyl)benzyl]
Thiosulfuric acid, H2S2O3, S-[α-[(dimethylamino)methyl]benzyl] esters, stereoisomers
Thiosulfuric acid, H2S2O3, S-[α-[1-(dimethylamino)ethyl]benzyl]
Thiosulfuric acid, H2S2O3, S-[α-[1-(methylamino)ethyl]benzyl] esters, stereoisomers
α-Toluenethiol, α-(aminomethyl)-, hydrogen sulfate (ester), DL-
α-Toluenethiol, α-(aminomethyl)-, DL-
α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, acetate (ester), erythro-
α-Toluenethiol, α-[1-(methylamino)ethyl]-, hydrogen sulfate (ester), threo-
IT Benzylamine, α-(1-chloroethyl)-
(N-alkyl derivs., stereochemistry of, nucleophilic rearrangements in relation to)
IT 645-62-5, 2-Hexenal, 2-ethyl-
(hydrogenation of, with Ni catalysts)
IT 936-42-5, Aziridine, 1,2-dimethyl-3-phenyl-, erythro- 936-43-6, Aziridine, 1,2-dimethyl-3-phenyl-, threo- 942-47-2, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, erythro- 945-44-8, Phenethylamine, β-methoxy-N,N,α-trimethyl-, hydrochloride, L(-)-erythro- 952-18-1, α-Toluenethiol, α-[(dimethylamino)methyl]-, hydrogen sulfate (ester), DL- 952-18-1, α-Toluenethiol, α-[(dimethylamino)methyl]-, hydrogen sulfate (ester), L(+)- 980-86-9, Benzylamine, α-(1-chloroethyl)-N-methyl-, picrate, threo- 1076-52-4, Benzylamine, α-(1-chloroethyl)-N-methyl-, hydrochloride, erythro- 1084-48-6, Ammonium, (β-mercapto-α-methylphenethyl)trimethyl, iodide, acetate, erythro- 1140-76-7, α-Toluenethiol, α-[1-(methylamino)ethyl]-, hydrogen sulfate (ester), erythro- 1165-97-5, Phenethylamine, β,β'-dithiobis[N,α-dimethyl-, dihydrochloride, erythro- 1201-46-3, Benzylamine, α-(1-chloroethyl)-N,N-dimethyl-, hydrochloride, erythro- **1210-30-6**, Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester, erythro- 1246-84-0, Benzylamine, α-(1-chloroethyl)-N,N-dimethyl-, picrate, erythro- 1444-33-3,

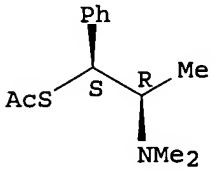
Phenethylamine, β,β'-dithiobis[N,α-dimethyl-, dipicrate, threo- 2202-60-0, Aziridine, 1,2-dimethyl-3-phenyl-, picrate, threo- 2202-61-1, Aziridine, 1,2-dimethyl-3-phenyl-, picrate, erythro- 2202-69-9, Benzyl alcohol, α-[(dimethylamino)methyl]-, L(+)- 2218-08-8, α-Toluenethiol, α-[(dimethylamino)methyl]-, L(+)- 2218-08-8, α-Toluenethiol, α-[(dimethylamino)methyl]-, DL- 2226-27-9, Acetamide, N-(β-mercapto-α-methylphenethyl)-N-methyl-, L-(-)-erythro- 2226-30-4, Phenethylamine, β,β'-dithiobis[N,α-dimethyl-, threo- 2226-31-5, Benzylamine, α-(1-chloroethyl)-N,N-dimethyl-, erythro- 2226-32-6, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, hydrogen sulfate (ester), erythro- 6853-14-1, Benzyl alcohol, α-[(dimethylamino)methyl]-, DL- 17605-71-9, Benzyl alcohol, α-[1-(dimethylamino)ethyl]-, DL- 65376-30-9, α-Toluenethiol, α-[1-(methylamino)ethyl]-, hydrochloride, threo- 69321-41-1, α-Toluenethiol, α-[1-(methylamino)ethyl]-, threo-
(preparation of)

IT **1210-30-6**, Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester, erythro-
(preparation of)

RN 1210-30-6 HCAPLUS

CN Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester, erythro- (8CI) (CA INDEX NAME)

Relative stereochemistry.



102 (b)

L40 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1965:8904 HCAPLUS

DN 62:8904

OREF 62:**1588a-c**

ED Entered STN: 22 Apr 2001

TI Phenylmercaptoalkylamines. III. Hofmann degradation of 1-phenyl-2-dimethylaminopropanethiol quaternary salts

AU Nishimura, Haruki; Takamatsu, Hideji

CS Dainippon Pharm. Co., Ltd., Osaka, Japan

SO Yakugaku Zasshi (**1964**), 84(9), 811-17
CODEN: YKKZAJ; ISSN: 0031-6903

DT Journal

LA Japanese

CC 35 (Noncondensed Aromatic Compounds)

AB Na2S2O3 and L-(+)-threo-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl, followed by hydrolysis, gave (+)-1-phenyl-2-dimethylaminopropanethiol (I), which was then converted into the methiodide and treated with NaOH to form (+)-1,2-epithiopropylbenzene (II), b10 100°, which was polymerized to give a polymer, m. 255-6°. Treatment of D-(+)-erythro-1,2-epoxypropylbenzene with KSCN gave L-(-)-erythro-1,2-epithiopropylbenzene, b7 92-3°, [α]20D -21.4° (c 2.21, MeOH), which was found to be the antipode of II. II belongs to the D-(+)-erythro series and I, to the L-(+)-threo series. The (-)-amino thiol, similarly derived from L-(-)-erythro-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl, was found to belong to the L-(-)-erythro series and that D-(+)-threo-1,2-epithiopropylbenzene (III) is derived from it. The steric configuration of II and III was also determined from their N.M.R. spectra. Hofmann degradation of the quaternary salt of 1-phenyl-2-dimethylaminoethanethiol

also gave the same result. II and III underwent desulfurization by heating to give trans-β-methylstyrene.

IT Elimination reactions
(Hofmann, of (β-mercaptophenethyl)trimethylammonium iodides)

IT Nuclear magnetic resonance
Stereochemistry
Stereochemistry
(of (1,2-epithiopropyl)benzenes and (1,2-epoxypropyl)benzenes)

IT Stereochemistry
(of α-(1-chloroethyl)benzylamine N-alkyl derivs.)

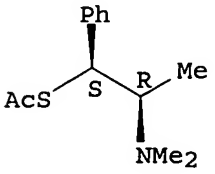
IT Spectra, visible and ultraviolet
(of D(+)-erythro- and -threo-(1,2-epoxypropyl)benzenes)

IT Acetic acid, thio-, S-esters with (β-mercaptophenethyl)trimethylammonium iodides
Ammonium, (β-mercapto-α-methylphenethyl)trimethyl, acetate, L-(+)-threo-
Ammonium, (β-mercapto-α-methylphenethyl)trimethyl, acetate, L-(-)-erythro-
Ammonium, (β-mercapto-α-methylphenethyl)trimethyl, L-(+)-threo-
Ammonium, (β-mercapto-α-methylphenethyl)trimethyl, L-(-)-erythro-
Benzylamine, α-(1-chloroethyl)-N-methyl-, hydrochloride, three-
Phenethylamine, β,β'-dithiobis[N,N,α-trimethyl-, dipicrate, L(+)-threo-
Phenethylamine, β,β'-dithiobis[N,N,α-trimethyl-, dipicrate, L(-)- erythro-
Phenethylamine, β,β'-dithiobis[N,N,α-trimethyl-, hydrochloride, L(+)-threo-
Phenethylamine, β,β'-dithiobis[N,N,α-trimethyl-, oxalate (1:2), L(-)-erythro-
Pseudourea, 2-[α-[1-(dimethylamino)ethyl]benzyl]-2-thio-, dipicrate, L(+)-threo-
Pseudourea, 2-[α-[1-(dimethylamino)ethyl]benzyl]-2-thio-, dipicrate, L(-)-erythro-
Thiazolidine, 3,4-dimethyl-5-phenyl-, picrate, L(-)-erythro-
Thiazolidine, 3,4-dimethyl-5-phenyl-, picrate, L(-)-threo-
Thiazolidine, 3,4-dimethyl-5-phenyl-, L(-)-erythro-
Thiazolidine, 3,4-dimethyl-5-phenyl-, L(-)-threo-
α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, acetate (ester), L(+)-threo-
α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, hydrochloride, L(-)-erythro-
α-Toluenethiol, α-[1-(methylamino)ethyl]-, hydrochloride, L(+)-threo-
α-Toluenethiol, α-[1-(methylamino)ethyl]-, L(+)-threo-

IT 942-50-7, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, hydrochloride, L(+)-threo- 1076-52-4, Benzylamine, α-(1-chloroethyl)-N-methyl-, hydrochloride, erythro- **1210-30-6**, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, acetate (ester), L(-)-erythro- **1210-30-6**, Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester, L(+)-threo- 1444-32-2, Pseudourea, 2-[α-[1-(dimethylamino)ethyl]benzyl]-2-thio-, dihydrochloride, L(+)-threo- 1498-99-3, Benzene, (epithioethyl)- 2218-22-6, Phenethylamine, β,β'-dithiobis[N,N,α-trimethyl-, L(-)-erythro- **2226-23-5**, Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester, L(-)-erythro- 2226-25-7, Phenethylamine, β,β'-dithiobis[N,N,α-trimethyl-, DL-threo- 4046-30-4, Pseudourea, 2-[α-[1-(dimethylamino)ethyl]benzyl]-2-thio-, dihydrochloride, L(-)-erythro- 94489-15-3, Ammonium, (β-mercaptophenethyl)trimethyl, iodide, DL- 94960-76-6, Phenethylamine, β,β'-dithiobis[α-methyl-, dihydrochloride, DL-threo- 96279-67-3, Ammonium, (β-mercaptophenethyl)trimethyl, iodide, acetate, DL-

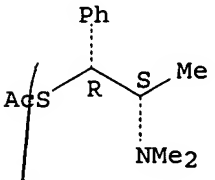
(preparation of)
IT 4518-66-5, Benzene, (1,2-epoxypropyl)-, D(+)-threo- 14212-53-4, Benzene, (1,2-epoxypropyl)-, D(+)-erythro-
(spectrum of)
IT 67921-36-2, Benzene, (1,2-epithiopropyl)-
(stereoisomers)
IT **1210-30-6**, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, acetate (ester), L(-)-erythro- **2226-23-5**, Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester, L(-)-erythro-
(preparation of)
RN 1210-30-6 HCAPLUS
CN Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester, erythro- (8CI) (CA INDEX NAME)

Relative stereochemistry.



RN 2226-23-5 HCAPLUS
CN Ethanethioic acid, S-[2-(dimethylamino)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L40 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1965:8902 HCAPLUS
DN 62:8902
OREF 62:**1587d-h**
ED Entered STN: 22 Apr 2001
TI Phenylmercaptoalkylamines. I. 1-Phenyl-2(or 3)-amino-alkanethiol derivatives
AU Nishimura, Haruki; Takamatsu, Hideji
CS Dainippon Pharm. Co., Ltd., Osaka, Japan
SO Yakugaku Zasshi (**1964**), 84(9), 797-805
CODEN: YKKZAJ; ISSN: 0031-6903
DT Journal
LA Japanese
CC 35 (Noncondensed Aromatic Compounds)
AB PhCH(OH)CH2R.HCl (1 part) is dissolved in 2 vols. CHCl3 and treated with a solution of SOCl2 (or PCl5) in CHCl3 under cooling to give the following PhCHClCH2R (I) (R, % yield, and m.p. of the hydrochloride given): NH2, 92, 164-5.5° (decomposition) (EtOH-Et2O); NHMe, 80, 175-6° (decomposition) (MeOH); NHEt, 63, 192° (decomposition) (iso-PrOH); NHPr, 94, 185-6° (iso-PrOH); iso-PrNH, 78, 185-6° (iso-PrOH); NMe2, 89, 206° (decomposition); NEt2, 100, --; NPr2, 48, 100.5-103° (AcOEt); iso-Pr2N, 55, 121-4° (AcOEt); pyrrolidino, 75, 181.5° (iso-PrOH); piperidino, 65, 178-9° (decomposition) (iso-PrOH); morpholino, 93, 188° (decomposition) (MeOH). Also prepared

are PhCHCl(CH2)2NMe2, m. 176°, and PhCHCl(CH2)2Z (Z = piperidino), m. 151°. Equimolar mixture of I.HCl and Na2S2O3.5H2O in 1-2 vols. H2O is boiled 30-60 min. to give the following PhCH(SSO3H)CH2R (II) [R and m.p. (decomposition) given]: NH2, 213-14°; NHMe, 184°; NHEt, 192°; NHPr, 201°; iso-PrNH, 192°; NMe2, 207°; NEt2, 178°; NPr2, 204°; iso-Pr2N, 204°; pyrrolidino, 187°; piperidino, 206°; morpholino, 221°. I is treated with NaSH or II is treated with HCl to give the following PhCH(SH)CH2R (III) (R, b.p./mm., and m.p. hydrochloride given): NH2, 116-20°/7, 157-60°; NHMe, 98-104°/6 (m. 67-9°), 129-33°; NHEt, 100°/4, 173°; NHPr, 115-17°/5-6, 163°; iso-PrNH, 102-4°/4, 175-7°; NMe2, 109-12°/5, 184-5° (decomposition); NEt2, 109-12°/5.5, --; NPr2, 122-8°/5, --; iso-Pr2N, 115-18°/5, 148-50°; pyrrolidino, 116-19°/4, 177.5-8.5°; piperidino, 131-3°/4, 179-80° (decomposition); morpholino, --, 192-3° (decomposition). Oxidation of III gives the following (RCH2CHPhS)2 (R and m.p. of the dihydrochloride given): NH2, 210-13°; NHMe, 190-3° (decomposition); NHEt, 187-90°; NHPr, 202-4°; iso-PrNH, 186-90°; NMe2, 211° (decomposition); NEt2, 205-7°; NPr2, 209-10° (decomposition); iso-Pr2N, -- [free base m. 80-1° (MeOH)]; pyrrolidino, -- [free base m. 102-5° (ligroine)]; piperidino, -- [free base m. 78-9° (MeOH)]; morpholino, 205-8°. Also prepared are: PhCH(SH)(CH2)2NMe2 (b8 109-10°); PhCH(SH)(CH2)2Z (b5 148-50.5°); [Me2N(CH2)2CHPhS]2 (picrate m. 85-90°), and [Z(CH2)2CHPhS]2 (picrate m. 95-100°).

IT Stereochemistry
(of 2-(alkylamino)-1-phenyl-1-propanethiols and related compds.)

IT Thiosulfuric acid, H2S2O3, S-[α-(aminomethyl)benzyl] esters

IT 934-14-5, α-Toluenethiol, α-(aminomethyl)- 939-51-5, Phenethylamine, β-chloro-N-ethyl-, hydrochloride 942-94-9, Benzyl alcohol, α-[(propylamino)methyl]- 952-20-5, α-Toluenethiol, α-[(ethylamino)methyl]-, hydrogen sulfate (ester) 952-49-8, Acetophenone, 2-(dipropylamino)- 952-52-3, 1-Piperidinepropanethiol, α-phenyl- 985-30-8, Morpholine, 4,4'-[thiobis(2-phenylethylene)]di- 985-55-7, Benzyl alcohol, α-[(diethylamino)methyl]-, picrate 985-81-9, Acetophenone, 2-(dipropylamino)-, picrate 986-81-2, Piperidine, 1,1'-[dithiobis(2-phenylethylene)]di- 988-62-5, Phenethylamine, β,β'-dithiobis[N,N-diisopropyl- 988-67-0, Piperidine, 1,1'-[dithiobis(3-phenyltrimethylene)]di- 1006-92-4, α-Toluenethiol, α-[(methylamino)methyl]- 1009-10-5, α-Toluenethiol, α-[(dimethylamino)methyl]-, hydrochloride 1009-15-0, Benzyl alcohol, α-[(ethylamino)methyl]-, hydrochloride 1009-16-1, α-Toluenethiol, α-[(ethylamino)methyl]- 1011-59-2, Propylamine, 3-chloro-N,N-dimethyl-3-phenyl-, hydrochloride 1011-63-8, Benzyl alcohol, α-[(propylamino)methyl]-, hydrochloride 1011-64-9, α-Toluenethiol, α-[(propylamino)methyl]- 1014-31-9, Benzyl alcohol, α-[(diethylamino)methyl]-, hydrochloride 1014-32-0, Pyrrolidine, 1-(β-chlorophenethyl)-, hydrochloride 1014-35-3, 1-Pyrrolidineethanethiol, α-phenyl-, hydrochloride 1017-25-0, 1-Piperidineethanethiol, α-phenyl- 1017-26-1, 1-Piperidineethanethiol, α-phenyl-, hydrochloride 1020-10-6, Phenethylamine, β-chloro-N,N-dipropyl-, hydrochloride 1020-11-7, Benzyl alcohol, α-[(dipropylamino)methyl]-, hydrochloride 1020-12-8, α-Toluenethiol, α-[(dipropylamino)methyl]- 1022-99-7, α-Toluenethiol, α-[(propylamino)methyl]-, hydrogen sulfate (ester) 1029-93-2, 4-Morpholineethanethiol, α-phenyl-, hydrogen sulfate (ester) 1078-35-9, Phenethylamine, β-chloro-N-isopropyl-, hydrochloride 1078-37-1, α-Toluenethiol, α-[(isopropylamino)methyl]- 1081-29-4, Pseudourea, 2-[α-[(dimethylamino)methyl]benzyl]-2-thio-, dihydrochloride 1083-08-5, Pseudourea, 2-[α-[2-(dimethylamino)ethyl]benzyl]-2-thio-,

dihydrochloride 1083-24-5, α-Toluenethiol, α-[(diisopropylamino)methyl]-, hydrochloride 1090-76-2, α-Toluenethiol, α-[(diisopropylamino)methyl]-, hydrogen sulfate (ester) 1094-81-1, Phenethylamine, β,β'-dithiobis[N-methyl-, dihydrochloride 1099-08-7, Phenethylamine, β,β'-dithiobis[N,N-dimethyl-, dihydrochloride 1102-17-6, Phenethylamine, β,β'-dithiobis[N-propyl-, dihydrochloride 1103-56-6, Pyrrolidine, 1,1'-[thiobis(2-phenylethylene)]di-, dihydrochloride 1104-61-6, Phenethylamine, β,β'-dithiobis[N,N-diethyl-, dihydrochloride 1111-14-4, Piperidine, 1,1'-[dithiobis(3-phenyltrimethylene)]di-, dipicrate 1131-81-3, α-Toluenethiol, α-[(isopropylamino)methyl]-, hydrochloride 1667-57-8, Morpholine, 4,4'-[thiobis(2-phenylethylene)]di-, dihydrochloride 2090-39-3, Phenethylamine, N,N-dimethyl-, picrate 2217-96-1, Benzyl alcohol, α-[(diisopropylamino)methyl]-, hydrochloride 2217-97-2, Phenethylamine, β-chloro-N-propyl-, hydrochloride 2217-98-3, Phenethylamine, β-chloro-N,N-diethyl- 2217-99-4, Phenethylamine, β-chloro-N,N-diisopropyl-, hydrochloride 2218-00-0, Morpholine, 4-(β-chlorophenethyl)-, hydrochloride 2218-01-1, α-Toluenethiol, α-(aminomethyl)-, hydrogen sulfate (ester) 2218-02-2, α-Toluenethiol, α-[(isopropylamino)methyl]-, hydrogen sulfate (ester) 2218-03-3, α-Toluenethiol, α-[(dipropylamino)methyl]-, hydrogen sulfate (ester) 2218-04-4, 1-Pyrrolidineethanethiol, α-phenyl-, hydrogen sulfate (ester) 2218-05-5, α-Toluenethiol, α-[(methylamino)methyl]-, hydrochloride 2218-06-6, α-Toluenethiol, α-[(ethylamino)methyl]-, hydrochloride 2218-07-7, α-Toluenethiol, α-[(propylamino)methyl]-, hydrochloride 2218-08-8, α-Toluenethiol, α-[(dimethylamino)methyl]- 2218-09-9, α-Toluenethiol, α-[(diethylamino)methyl]- 2218-10-2, α-Toluenethiol, α-[(diisopropylamino)methyl]- 2218-11-3, 1-Pyrrolidineethanethiol, α-phenyl- 2218-12-4, 4-Morpholineethanethiol, α-phenyl-, hydrochloride 2218-13-5, Acetophenone, 2-(diisopropylamino)- 2218-14-6, Acetophenone, 2-(diisopropylamino)-, hydrochloride 2218-15-7, Acetophenone, 2-(1-pyrrolidinyl)- 2218-16-8, Acetophenone, 2-(1-pyrrolidinyl)-, hydrochloride 2218-17-9, Pyrrolidine, 1,1'-[thiobis(2-phenylethylene)]di- 2218-18-0, Pyrrolidine, 1,1'-[dithiobis(2-phenylethylene)]di- 2218-19-1, α-Toluenethiol, α-[2-(dimethylamino)ethyl]- 3852-66-2, α-Toluenethiol, α-(aminomethyl)-, hydrochloride 3907-60-6, Phenethylamine, β,β'-dithiobis-, dihydrochloride 3907-61-7, Phenethylamine, β,β'-dithiobis[N-ethyl-, dihydrochloride 3907-62-8, Phenethylamine, β,β'-dithiobis[N-isopropyl-, dihydrochloride 3907-63-9, Phenethylamine, β,β'-dithiobis[N,N-dipropyl-, dihydrochloride 3907-64-0, Pseudourea, 2-[α-(piperidinomethyl)benzyl]-2-thio-, dihydrochloride 4046-29-1, Morpholine, 4,4'-[dithiobis(2-phenylethylene]di-, dihydrochloride 4047-56-7, Pseudourea, 2-[α-(2-piperidinoethyl)benzyl]-2-thio-, dihydrochloride 4309-59-5, Phenethylamine, β,β'-thiobis[N,N-diisopropyl-, dihydrochloride 4599-02-4, Benzyl alcohol, α-[(dipropylamino)methyl]-, picrate 10275-21-5, Phenethylamine, N,N-dimethyl-, hydrochloride (preparation of)

L40 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1961:13367 HCAPLUS
DN 55:13367
OREF 55:**2616e**
ED Entered STN: 22 Apr 2001
TI Cyclization of N-allylthioamides and their homologs with particular attention to thiazoline synthesis
AU Sullivan, John M.
CS Univ. of Michigan, Ann Arbor

SO (1960) 57 pp. Avail.: Univ. Microfilms (Ann Arbor, Mich.), Order No. 60-2575
From: Dissertation Abstr. 20, 297
DT Dissertation
LA Unavailable
CC 10G (Organic Chemistry: Heterocyclic Compounds)
OS CASREACT 55:13367
AB Unavailable
IT Ring closure or formation
(of N-allylthioamides, thiazolines by)
IT Amides
(N-allylthio, cyclization to thiazolines)
IT 31152-37-1, Thiazoline
(derivs., formation from N-allylthioamides)

=> d all hitstr tot l41

L41 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:497835 HCAPLUS
DN 131:350834
ED Entered STN: 11 Aug 1999
TI Utilization of industrial waste materials. Part 14. Synthesis of β-amino alcohols and thiols with a 2-azabicyclo[3.3.0]octane backbone and their application in enantioselective catalysis
AU Kossenjans, Michael; Soeberdt, Michael; Wallbaum, Sabine; Harms, Klaus; Martens, Jurgen; Aurich, Hans Gunter
CS Fachbereich Chemie, Universitat Oldenburg, Oldenburg, D-26129, Germany
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (16), 2353-2365
CODEN: JCPRB4; ISSN: 0300-922X
PB Royal Society of Chemistry
DT Journal
LA English
CC ~~21-2~~ (General Organic Chemistry)
Section cross-reference(s): 25, 75
OS CASREACT 131:350834
AB New, chiral β-tert-amino tert-alcs. were synthesized from an enantiomerically pure sec-amine via glycine, alanine and phenylglycine derivs. Grignard addns. to these esters provided rigid amino alcs. in fair yields. The absolute configurations of the stereogenic centers, which arose during the alkylation step, were assigned by an independent route leading to some of the optical antipodes. The target compds. were derivs. of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol. Condensation of enantiomerically pure β-amino alcs. with a γ-keto ester afforded N,O-acetals which were subsequently reduced to the β-tert-amino alcs. X-Ray anal. of one compound was performed to verify the stereochem. observed by chemical correlation. The nucleophilic ring opening of enantiomerically pure styrene oxide by an amine resulted in the formation of regioisomeric amino alcs. Amino thiol derivs. were also prepared Reduction of these compds. to thiols and subsequent oxidation afforded
amino disulfides. Finally, the bicyclic β-amino alcs. and thiols were used as chiral **ligands** in the enantioselective addition of diethylzinc to benzaldehyde and ee values up to 96% were found.
ST stereoselective addn catalyst amino alc thiol; oxaazatricycloundecanone prepn crystal mol structure
IT Alcohols, preparation
Thiols (organic), preparation
Thiols (organic), preparation
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(amino; preparation of cyclopenta[b]pyrrole-1-ethanol and

cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

IT Crystal structure
Molecular structure
(preparation and properties of oxaazatricycloundecanone)

IT Stereochemistry
(preparation of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

IT **Addition reaction**
Addition reaction catalysts
(stereoselective; preparation of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

IT Amines, preparation
Amines, preparation
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(thiol; preparation of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

IT 613-87-6P, (S)-1-Phenyl-1-propanol 1565-74-8P, (R)-1-Phenyl-1-propanol
206264-72-4P 206264-79-1P 206264-81-5P 250371-07-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 180624-37-7P 250371-06-3P 250371-09-6P 250371-12-1P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

IT 156366-41-5P 206264-68-8P 206264-70-2P 206264-74-6P 206264-77-9P
250370-87-7P 250370-88-8P 250370-89-9P 250370-90-2P 250370-91-3P
250370-92-4P 250370-93-5P 250370-94-6P 250370-95-7P 250370-96-8P
250370-97-9P 250370-98-0P 250370-99-1P 250371-00-7P 250371-01-8P
250371-02-9P 250371-03-0P 250371-10-9P 250371-11-0P 250371-14-3P
250371-17-6P 250371-20-1P 250371-22-3P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

IT 250371-08-5P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

IT 100-52-7, Benzaldehyde, reactions 492-41-1 557-20-0, Diethylzinc
930-68-7, 2-Cyclohexen-1-one 2026-48-4 2749-11-3 3182-95-4
5445-17-0, 2-Bromopropanoic acid methyl ester 20780-53-4 20780-54-5
20826-94-2, 2-Oxocyclopentaneacetic acid ethyl ester 74004-88-9,
α-Bromobenzeneacetic acid phenylmethyl ester 78603-91-5
79868-78-3 128900-19-6 156473-27-7 161779-74-4 250371-29-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

IT 161779-72-2P 206264-50-8P 206264-54-2P 206264-57-5P 206264-60-0P
206264-66-6P 250370-83-3P 250370-84-4P 250370-85-5P 250370-86-6P
250371-05-2P 250371-35-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD
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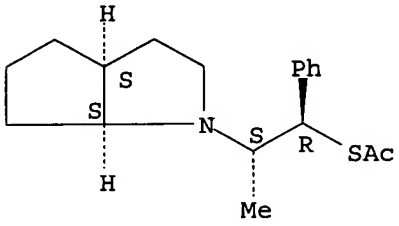
IT **250371-17-6P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

RN 250371-17-6 HCAPLUS
CN Ethanethioic acid, S-[(1R,2S)-2-[(3aS,6aS)-hexahydrocyclopenta[b]pyrrol-1(2H)-yl]-1-phenylpropyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



102

L41 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:569540 HCAPLUS
DN 129:289723
ED Entered STN: 08 Sep 1998
TI Zirconocene-**Zinc** Transmetalation and in Situ Catalytic Asymmetric Addition to **Aldehydes**
AU Wipf, Peter; Ribe, Seth
CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA
SO Journal of Organic Chemistry (**1998**), 63(19), 6454-6455
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 21-2 (General Organic Chemistry)
AB The in situ hydrozirconation of alkynes, trans-metalation to dimethylzinc and chiral amino thiol-catalyzed addition to **aldehydes** provided an efficient protocol for the asym. preparation of (E)-allylic alcs. For example, the hydrozirconation of 1-hexyne, followed by transmetalation via addition of dimethylzinc and sequential addition of the resulting (alkenyl)methylzinc intermediate to benzaldehyde gave [S-(E)]-1-phenyl-2-hepten-1-ol [i.e., [S-(E)]-α-(1-hexenyl)benzenemethanol] in 90% and in 83% enantiomeric excess. The last step in the sequence was catalyzed in the presence of (R)-2-[1-(dimethylamino)propyl]benzenethiol as **ligand.**
ST allylic alc prepn; hydrozirconation transmetalation addn **aldehyde**
IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(allyl; preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to **aldehydes**)
IT **Aldehydes**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aromatic; preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to **aldehydes**)
IT **Hydrometalation**
(hydrozirconation; preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to **aldehydes**)
IT Stereochemistry

Transmetalation
(preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to **aldehydes**)

IT **Aldehydes**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to **aldehydes**)

IT **Addition reaction**
(stereoselective; preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to **aldehydes**)

IT 37342-97-5, Zirconocene hydride chloride 103729-96-0 112068-01-6 114389-70-7 135190-26-0 **185606-94-4**
RL: CAT (Catalyst use); USES (Uses)
(preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to **aldehydes**)

IT 214214-54-7P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to **aldehydes**)

IT 100-52-7, Benzaldehyde, reactions 104-53-0, Hydrocinnamaldehyde 104-88-1, 4-Chlorobenzaldehyde, reactions 123-11-5, 4-Methoxybenzaldehyde, reactions 455-19-6, 4-(Trifluoromethyl)benzaldehyde 544-97-8, Dimethylzinc 591-31-1, 3-Methoxybenzaldehyde 693-02-7, 1-Hexyne 917-92-0, 3,3-Dimethyl-1-butyne 928-49-4, 3-Hexyne 2043-61-0, Cyclohexanecarboxaldehyde 3082-64-2, (R)-α-Ethylbenzylamine 214214-55-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to **aldehydes**)

IT 214214-53-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to **aldehydes**)

IT 140148-19-2P 140148-22-7P 214214-56-9P 214214-57-0P 214214-58-1P 214214-59-2P 214214-60-5P 214214-61-6P 214214-62-7P 214214-63-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to **aldehydes**)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

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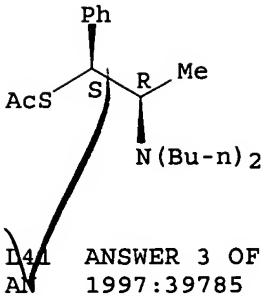
IT **185606-94-4**
RL: CAT (Catalyst use); USES (Uses)
(preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to **aldehydes**)

RN 185606-94-4 HCAPLUS
CN Ethanethioic acid, S-[(1S,2R)-2-(dibutylamino)-1-phenylpropyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



102 (b)

L41 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:39785 HCAPLUS
DN 126:131036
ED Entered STN: 18 Jan 1997
TI Chiral β-amino thiol catalysts for the enantioselective addition of diethylzinc to **aldehydes**
AU Kang, Jahyo; Kim, Jeong Whan; Lee, Jun Won; Kim, Dong Soo; Kim, Joo In
CS Dep. Chem., Sogang Univ., Seoul, 121-742, S. Korea
SO Bulletin of the Korean Chemical Society (**1996**), 17(12), 1135-1142
CODEN: BKCSDE; ISSN: 0253-2964
PB Korean Chemical Society
DT Journal
LA English
CC 21-2 (General Organic Chemistry)
AB Reaction of diethylzinc with α-branched **aldehydes** in the presence of a catalytic amount (5 mol %) of various β-amino thiols in toluene or ether provided the corresponding secondary alcs. in outstanding ee. Detailed preparative procedure for the β-amino thiols are presented.
ST enantioselective addn diethylzinc **aldehyde** thiol catalyst
IT Stereochemistry
(enantioselective addition of diethylzinc to **aldehydes** using chiral β-amino thiol catalysts)
IT **Aldehydes**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective addition of diethylzinc to **aldehydes** using chiral β-amino thiol catalysts)
IT **Addition reaction**
Addition reaction catalysts
(stereoselective; enantioselective addition of diethylzinc to **aldehydes** using chiral β-amino thiol catalysts)
IT 160011-80-3P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(enantioselective addition of diethylzinc to **aldehydes** using chiral β-amino thiol catalysts)
IT 160011-81-4P 166031-49-8P 166031-50-1P 166031-51-2P 166031-52-3P 166031-53-4P 186314-12-5P 186314-14-7P 186314-16-9P 186314-20-5P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(enantioselective addition of diethylzinc to **aldehydes** using chiral β-amino thiol catalysts)
IT 66-25-1, Hexanal 66-77-3, 1-Naphthalenecarboxaldehyde 66-99-9, 2-Naphthalenecarboxaldehyde 100-52-7, Benzaldehyde, reactions 104-88-1, 4-Chlorobenzaldehyde, reactions 111-24-0, 1,5-Dibromopentane 123-11-5, 4-Methoxybenzaldehyde, reactions 135-02-4, 2-Methoxybenzaldehyde 459-57-4, 4-Fluorobenzaldehyde 492-41-1, (1R,2S)-Norephedrine 498-66-8, Bicyclo[2.2.1]hept-2-ene 557-20-0, Diethylzinc 630-19-3, Pivaldehyde 2043-61-0, Cyclohexanecarboxaldehyde 12093-10-6, Ferrocenecarboxaldehyde 14371-10-9, trans-Cinnamaldehyde 23190-16-1 38274-14-5, 2,2'-Bis(bromomethyl)-1,1'-biphenyl
RL: RCT (Reactant); RACT (Reactant or reagent)

(enantioselective addition of diethylzinc to **aldehydes** using chiral β-amino thiol catalysts)

IT 3965-56-8P 10283-91-7P 58066-43-6P 70492-66-9P, (R)-Octan-3-ol
111138-85-3P 115651-77-9P 127641-25-2P 133576-76-8P 141623-44-1P
160011-79-0P 160167-27-1P 166031-42-1P 166031-43-2P
166031-44-3P **166031-45-4P** 166031-46-5P 166031-47-6P
166031-48-7P 186314-10-3P **186314-11-4P** 186314-13-6P
186314-15-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective addition of diethylzinc to **aldehydes** using chiral β-amino thiol catalysts)

IT 1565-74-8P 83740-16-3P 105836-13-3P 105836-14-4P 110558-24-2P
110611-21-7P 110611-22-8P 112576-12-2P 114091-67-7P 166031-40-9P
166031-54-5P 166371-89-7P 186314-09-0P 186314-18-1P
186314-19-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective addition of diethylzinc to **aldehydes** using chiral β-amino thiol catalysts)

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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(2) Capillon, J; Tetrahedron 1979, V35, P1817 HCAPLUS
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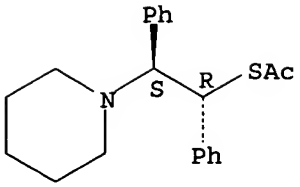
IT **160011-79-0P** **166031-44-3P** **166031-45-4P**
166031-48-7P **186314-11-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective addition of diethylzinc to **aldehydes** using chiral β-amino thiol catalysts)

RN 160011-79-0 HCAPLUS
CN Ethanethioic acid, S-[1,2-diphenyl-2-(1-piperidinyl)ethyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

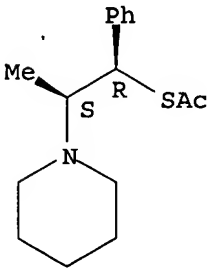
Absolute stereochemistry. Rotation (-).



102(b)

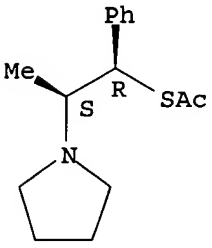
RN 166031-44-3 HCAPLUS
CN Ethanethioic acid, S-[1-phenyl-2-(1-piperidinyl)propyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 166031-45-4 HCAPLUS
CN Ethanethioic acid, S-[1-phenyl-2-(1-pyrrolidinyl)propyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

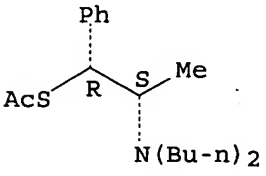
Absolute stereochemistry.



102(b)

RN 166031-48-7 HCAPLUS
CN Ethanethioic acid, S-[2-(dibutylamino)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

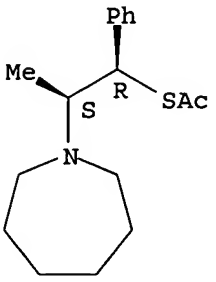
Absolute stereochemistry.



102(b)

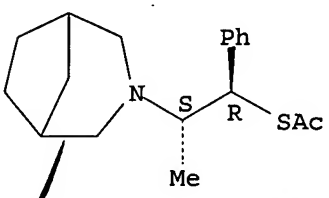
RN 186314-11-4 HCAPLUS
CN Ethanethioic acid, S-[2-(hexahydro-1H-azepin-1-yl)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **186314-19-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective addition of diethylzinc to **aldehydes** using chiral β-amino thiol catalysts)
RN 186314-19-2 HCAPLUS
CN Ethanethioic acid, S-[2-(3-azabicyclo[3.2.1]oct-3-yl)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

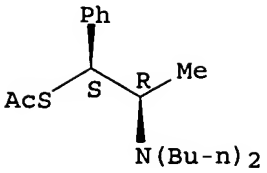
Absolute stereochemistry.



L41 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:729946 HCAPLUS
DN 126:103872
ED Entered STN: 12 Dec 1996
TI New chiral catalysts for the highly enantioselective addition of diethylzinc to **aldehydes**
AU Jin, Myung-Jong; Ahn, Sum-Jin; Lee, Kyoung-Soo
CS Dep. Chemical Engineering, Inha Univ., Inchon, 402-751, S. Korea
SO Tetrahedron Letters (**1996**), 37(48), 8767-8770
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier
DT Journal
LA English
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
AB Optically active amino thioacetate derivs. of (+)-norephedrine were found to act as effective catalysts for enantioselective addition of diethylzinc to **aldehydes**. This reaction provided optically active secondary alcs. with e.e. of up to >99%.
ST chiral catalyst stereoselective addn ethylzinc **aldehyde**; alc secondary chiral prepn
IT **Addition reaction**
Asymmetric synthesis and induction
Stereochemistry
Transition state structure
(chiral catalysts for enantioselective addition of diethylzinc to **aldehydes**)
IT **Aldehydes**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(chiral catalysts for enantioselective addition of diethylzinc to

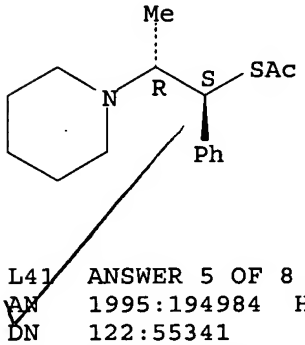
aldehydes)
IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(secondary, chiral; chiral catalysts for enantioselective addition of diethylzinc to **aldehydes**)
IT Catalysts
RL: CAT (Catalyst use); USES (Uses)
(stereoselective; chiral catalysts for enantioselective addition of diethylzinc to **aldehydes**)
IT **185606-94-4 185606-97-7**
RL: CAT (Catalyst use); USES (Uses)
(chiral catalysts for enantioselective addition of diethylzinc to **aldehydes**)
IT 66-99-9, 2-Naphthalenecarboxaldehyde 100-52-7, Benzaldehyde, reactions 104-88-1, 4-Chlorobenzaldehyde, reactions 123-11-5, 4-Methoxybenzaldehyde, reactions 135-02-4, 2-Methoxybenzaldehyde 2043-61-0, Cyclohexanecarboxaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(chiral catalysts for enantioselective addition of diethylzinc to **aldehydes**)
IT 613-87-6P 73854-04-3P 73890-73-0P 87241-23-4P 110529-28-7P 114389-71-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 25267-27-0, Iodobutane 37577-28-9, (+)-Norephedrine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of chiral catalysts for enantioselective addition of diethylzinc
to **aldehydes**)
IT 114389-70-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral catalysts for enantioselective addition of diethylzinc
to **aldehydes**)
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Corey, E; Tetrahedron Lett 1987, V28, P5237 HCAPLUS
(2) Hof, R; Tetrahedron:Asymmetry 1994, V5, P31 HCAPLUS
(3) Jones, G; Tetrahedron:Asymmetry 1993, V4, P261 HCAPLUS
(4) Kang, J; J Chem Soc, Chem Comm 1994, P2009 HCAPLUS
(5) Kitamura, M; J Am Chem Soc 1986, V108, P6071 HCAPLUS
(6) Kitamura, M; J Am Chem Soc 1989, V111, P4028 HCAPLUS
(7) Noyori, R; Angew Chem Int Ed Engl 1991, V30, P49
(8) Noyori, R; Asymmetric Catalysis in Organic Synthesis 1993
(9) Oguni, N; Tetrahedron Lett 1984, V25, P2823 HCAPLUS
(10) Rosini, C; Tetrahedron:Asymmetry 1991, V2, P363 HCAPLUS
(11) Soai, K; Bull Chem Soc Jpn 1989, V62, P2124 HCAPLUS
(12) Soai, K; Chem Rev 1992, V92, P833 HCAPLUS
(13) Soai, K; J Am Chem Soc 1987, V109, P7111 HCAPLUS
(14) Soai, K; J Org Chem 1991, V56, P4264 HCAPLUS
IT **185606-94-4 185606-97-7**
RL: CAT (Catalyst use); USES (Uses)
(chiral catalysts for enantioselective addition of diethylzinc to **aldehydes**)
RN 185606-94-4 HCAPLUS
CN Ethanethioic acid, S-[(1S,2R)-2-(dibutylamino)-1-phenylpropyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



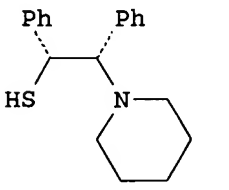
RN 185606-97-7 HCAPLUS
CN Ethanethioic acid, S-[1-phenyl-2-(1-piperidinyl)propyl] ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

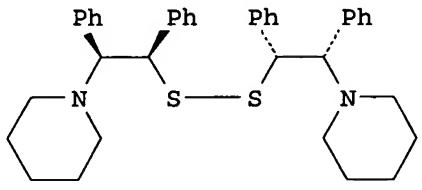


102(b)

L41 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:194984 HCAPLUS
DN 122:55341
ED Entered STN: 17 Nov 1994
TI Enantioselective addition of diethylzinc to **aldehydes** catalyzed by a drug-unrelated chiral amino thiol and the corresponding disulfide
AU Kang, Jahyo; Kim, Dong Soo; Kim, Joo In
CS Department Chemistry, Sogang University, Seoul, 121-742, S. Korea
SO Synlett (**1994**), (10), 842-4
CODEN: SYNLES; ISSN: 0936-5214
PB Thieme
DT Journal
LA English
CC 21-2 (General Organic Chemistry)
OS CASREACT 122:55341
GI



I



II

AB Reaction of diethylzinc with **aldehydes** in the presence of a catalytic amount of a β-amino thiol I (5 mol %) and the disulfide II (2.5 mol %) in toluene at 0° provided the corresponding secondary alcs. in excellent ee's.
ST diethylzinc stereoselective addn **aldehyde**; phenylpiperidinylpropanethiol catalyst stereoselective addn **aldehyde**; phenylpiperidinylpropyl disulfide catalyst stereoselective addn **aldehyde**; alc stereoselective prepn
IT Stereochemistry
(enantioselective addition of diethylzinc with **aldehydes**

catalyzed by chiral amino thiol and disulfide)

IT **Aldehydes**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective addition of diethylzinc with **aldehydes** catalyzed by chiral amino thiol and disulfide)

IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective addition of diethylzinc with **aldehydes** catalyzed by chiral amino thiol and disulfide)

IT **Addition reaction**
Addition reaction catalysts
(stereoselective, enantioselective addition of diethylzinc with **aldehydes** catalyzed by chiral amino thiol and disulfide)

IT 160011-80-3P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(enantioselective addition of diethylzinc with **aldehydes** catalyzed by chiral amino thiol and disulfide)

IT 160011-81-4P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(enantioselective addition of diethylzinc with **aldehydes** catalyzed by chiral amino thiol and disulfide)

IT 66-25-1, Hexanal 66-99-9, Naphthalene-2-carboxaldehyde 100-52-7, Benzaldehyde, reactions 104-88-1, 4-Chlorobenzaldehyde, reactions 123-11-5, 4-Methoxybenzaldehyde, reactions 135-02-4, 2-Methoxybenzaldehyde 557-20-0, Diethyl **zinc** 630-19-3, 2,2-Dimethylpropanal 2043-61-0, Cyclohexanecarboxaldehyde 12093-10-6, Ferrocenecarboxaldehyde 14371-10-9, trans-Cinnamaldehyde 23190-16-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective addition of diethylzinc with **aldehydes** catalyzed by chiral amino thiol and disulfide)

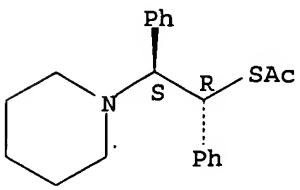
IT **160011-79-0P** 160167-27-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective addition of diethylzinc with **aldehydes** catalyzed by chiral amino thiol and disulfide)

IT 1565-74-8P 38636-36-1P 38636-38-3P 70492-66-9P 83740-16-3P 105836-13-3P 105836-14-4P 110611-21-7P 110611-22-8P 112576-12-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective addition of diethylzinc with **aldehydes** catalyzed by chiral amino thiol and disulfide)

IT **160011-79-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective addition of diethylzinc with **aldehydes** catalyzed by chiral amino thiol and disulfide)

RN 160011-79-0 HCAPLUS
CN Ethanethioic acid, S-[1,2-diphenyl-2-(1-piperidinyl)ethyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L41 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:86424 HCAPLUS
DN 123:142957
ED Entered STN: 08 Nov 1994
TI Enantioselective addition of diethylzinc to α-branched **aldehydes**
AU Kang, Jahyo; Lee, Jun Won; Kim, Joo In
CS Department of Chemistry, Sogang University, Seoul, 121-742, S. Korea
SO Journal of the Chemical Society, Chemical Communications (**1994**), (17), 2009-10
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
CC 21-2 (General Organic Chemistry)
AB Reaction of diethylzinc with α-branched **aldehydes** in the presence of a catalytic amount of (1R,2S)-(-)-1-phenyl-2-piperidinopropane-1-thiol provided the corresponding secondary alcs. in almost 100% enantiomeric excess.
ST enantioselective addn diethylzinc branched **aldehyde**
IT Optimization
(for enantioselective addition of diethylzinc to α-branched **aldehydes**)
IT Asymmetric synthesis and induction
(in enantioselective addition of diethylzinc to α-branched **aldehydes**)
IT **Aldehydes**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(α-branched; enantioselective addition of diethylzinc to α-branched **aldehydes**)
IT **Addition reaction catalysts**
(β-amino thiols stereoselective; for enantioselective addition of diethylzinc to α-branched **aldehydes**)
IT **Ligands**
RL: CAT (Catalyst use); USES (Uses)
(β-amino thiols; for enantioselective addition of diethylzinc to α-branched **aldehydes**)
IT **Aldehydes**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aryl, enantioselective addition of diethylzinc to α-branched **aldehydes**)
IT 166031-50-1P 166031-51-2P 166031-52-3P 166031-53-4P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(as **ligand** catalyst for enantioselective addition of diethylzinc to α-branched **aldehydes**)
IT 166031-49-8P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(best catalyst; as **ligand** catalyst for enantioselective addition of diethylzinc to α-branched **aldehydes**)
IT 91-13-4, 1,2-Bis(bromomethyl)benzene 109-65-9, Butyl bromide 110-52-1, 1,4-Dibromobutane 111-24-0, 1,5-Dibromopentane 492-41-1 10387-40-3, Potassium thioacetate 38274-14-5, 2,2'-Bis(bromomethyl)biphenyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(conversion to **ligand** catalyst for enantioselective addition of diethylzinc to α-branched **aldehydes**)
IT 166031-40-9P 166031-41-0P 166031-54-5P
RL: PNU (Preparation, unclassified); PREP (Preparation)
(enantioselective addition of diethylzinc to α-branched **aldehydes**)
IT 66-25-1, Hexanal 66-77-3, 1-Naphthaldehyde 66-99-9, 2-Naphthaldehyde 100-52-7, Benzaldehyde, reactions 104-88-1, 4-Chlorobenzaldehyde, reactions 123-11-5, 4-Methoxybenzaldehyde, reactions 135-02-4,

2-Methoxybenzaldehyde 459-57-4, 4-Fluorobenzaldehyde 557-20-0, Diethylzinc 630-19-3, Pivalaldehyde 2043-61-0, Cyclohexanecarboxaldehyde 12093-10-6, Ferrocenylcarboxaldehyde 14371-10-9, trans-Cinnamaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective addition of diethylzinc to α-branched **aldehydes**)

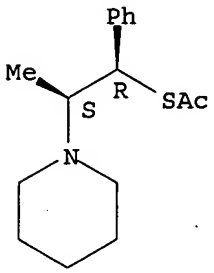
IT 1565-74-8P 38636-36-1P 38636-38-3P 70492-66-9P 83740-16-3P 105836-13-3P 105836-14-4P 110611-21-7P 110611-22-8P 112576-12-2P 114091-67-7P 166371-89-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective addition of diethylzinc to α-branched **aldehydes**)

IT 115651-77-9P 127641-25-2P 133576-76-8P 166031-42-1P 166031-43-2P **166031-44-3P 166031-45-4P** 166031-46-5P 166031-47-6P **166031-48-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthetic intermediate; in conversion to **ligand** catalyst for enantioselective addition of diethylzinc to α-branched **aldehydes**)

IT **166031-44-3P 166031-45-4P 166031-48-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthetic intermediate; in conversion to **ligand** catalyst for enantioselective addition of diethylzinc to α-branched **aldehydes**)

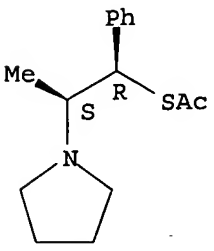
RN 166031-44-3 HCAPLUS
CN Ethanethioic acid, S-[1-phenyl-2-(1-piperidinyl)propyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 166031-45-4 HCAPLUS
CN Ethanethioic acid, S-[1-phenyl-2-(1-pyrrolidinyl)propyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

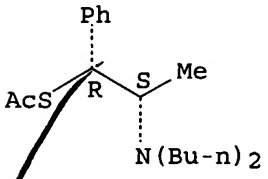
Absolute stereochemistry.



RN 166031-48-7 HCAPLUS

CN Ethanethioic acid, S-[2-(dibutylamino)-1-phenylpropyl] ester, [R-(R*,S*)]-(9CI) (CA INDEX NAME)

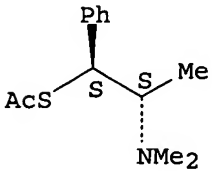
Absolute stereochemistry.



L41 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:680925 HCAPLUS
DN 121:280925
ED Entered STN: 10 Dec 1994
TI Nucleophilic substitutions using O-alkyl-N,N'-dialkylisoureas. Applications to ephedrines
AU Poelert, Martin A.; Hulshof, L. A.; Kellogg, Richard M.
CS Dep. Organic Chemi., Univ. Groningen, Groningen, 9747 AG, Neth.
SO Recueil des Travaux Chimiques des Pays-Bas (**1994**), 113(7-8), 365-8
CODEN: RTCPA3; ISSN: 0165-0513
DT Journal
LA English
CC 31-2 (Alkaloids)
Section cross-reference(s): 22
OS CASREACT 121:280925
AB Dialkylcarbodiimides in the presence of a CuI catalyst react cleanly with the hydroxyl group of N-methylated (1R,2S)-ephedrine and (1S,2S)-pseudoephedrine. These adducts react with nucleophiles like alkyl and aryl thiols as well as thioic acids and phthalimide to form the substitution products with overall retention of configuration. It is postulated that intramol. participation of the amino group via an SN2 reaction leads to aziridinium salts, which are subsequently opened by the nucleophiles via a second SN2 reaction. This synthetic approach is also useful for the inversion of simple secondary alcs.; on treatment with dicyclohexylcarbodiimide followed by benzothioic acid and treatment with LiAlH4, menthol was converted in good yield to neomenthane thiol.
ST nucleophilic substitution alkyldialkylisourea ephedrine; isourea alkyldialkyl nucleophilic substitution
IT Substitution reaction, nucleophilic
(nucleophilic substitutions using alkyldialkylisoureas, applications to ephedrines)
IT 85-41-6, Phthalimide 90-82-4, (1S,2S)-Pseudoephedrine 108-98-5, Benzenethiol, reactions 299-42-3 552-79-4, (1R,2S)-N-Methylephedrine 693-13-0, Diisopropylcarbodiimide 51018-28-1, (1S,2S)-N-Methylpseudoephedrine 86408-07-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(nucleophilic substitutions using alkyldialkylisoureas, applications to ephedrines)
IT 2218-22-6P 158837-58-2P 158837-60-6P 158837-61-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(nucleophilic substitutions using alkyldialkylisoureas, applications to ephedrines)
IT **2226-22-4P 2226-23-5P** 53273-24-8P 116588-21-7P 139528-47-5P 158837-59-3P 158837-62-8P 158837-63-9P 158837-64-0P 158837-65-1P 158931-23-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(nucleophilic substitutions using alkyldialkylisoureas, applications to

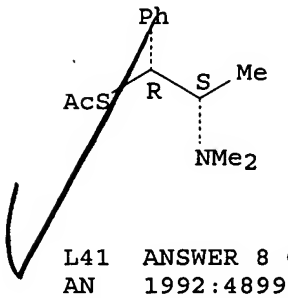
ephedrines)
IT **2226-22-4P 2226-23-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(nucleophilic substitutions using alkyldialkylisoureas, applications to ephedrines)
RN 2226-22-4 HCAPLUS
CN Ethanethioic acid, S-[2-(dimethylamino)-1-phenylpropyl] ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

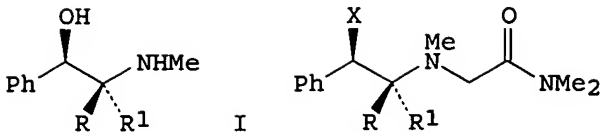


RN 2226-23-5 HCAPLUS
CN Ethanethioic acid, S-[2-(dimethylamino)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

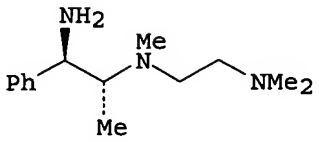


L41 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:489920 HCAPLUS
DN 117:89920
ED Entered STN: 05 Sep 1992
TI Stereo- and regioselective synthesis of chiral diamines and triamines from pseudoephedrine and ephedrine
AU Dieter, R. Karl; Deo, Niranjan; Lagu, Bharat; Dieter, Janice W.
CS Dep. Chem., Clemson Univ., Clemson, SC, 29634-1905, USA
SO Journal of Organic Chemistry (**1992**), 57(6), 1663-71
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
OS CASREACT 117:89920
GI



I

II



III

AB N-alkylated derivs. of (1R,2R)-(-)-pseudoephedrine and (1R,2S)-(-)-ephedrine give upon reaction with methanesulfonyl chloride, mixts. of 1-chloro- and 2-chloroamines which undergo stereoselective and regioselective substitution reactions with NaN3, amine, imides, thiols, thiolacetic acid, N-hydroxyphthalimide, and Ph2PH to give, in each case, a single isomeric product. These substitution reactions proceed with net retention of configuration. The procedure is not readily extended to nonbenzylic systems which give widely varying yields and regioisomeric ratios. The methodol. provides for a facile synthesis of chiral diamines, triamines, aminohydroxylamines, aminothiols, aminosulfides, and aminophosphines from chiral 1,2-amino alcs. wherein either the amine or alc. functionality is benzylic. Thus, treating pseudophedrine I (R = H, R1 = Me) with ClCH2CONMe2 gave 84% amide II (X = OH) which was sequentially treated with MeSO2Cl and NaN3 to give 70% azides II (X = N3). Reduction of the latter by LiAlH4 gave 60% triamine III. Analogous results were obtained with ephedrine I (R = Me, R1 = H).

ST pseudoephedrine regioselective stereoselective nucleophile reaction; ephedrine regioselective stereoselective nucleophile reaction; chiral synthesis diamine triamine; amine di pseudoephedrine chiral synthesis; substitution ephedrine pseudoephedrine stereochem regiochem; aminohydroxyl amine regiochem stereochem synthesis; aminothiol regiochem stereochem synthesis; aminosulfide regiochem stereochem synthesis; aminophosphine regiochem synthesis

IT Imides
Imines
Thiols, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(nucleophilic substitution by, of N-alkylated derivs. of pseudoephedrine and ephedrine)

IT Regiochemistry
Stereochemistry
(of nucleophilic substitution reactions of, N-alkylated derivs. of pseudoephedrine and ephedrine)

IT Substitution reaction, nucleophilic
(of N-alkylated derivs. pseudoephedrine and ephedrine by sodium azide, amines, imides, and thiols)

IT Nucleophiles
(regio- and stereoselective substitution by, of N-alkylated derivs. of pseudoephedrine and ephedrine)

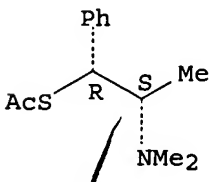
IT 2675-89-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of pseudoephedrine and ephedrine)

IT 62-53-3, Aniline, reactions 108-91-8, Cyclohexanamine, reactions 109-73-9, Butylamine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of ephedrine and pseudoephedrine derivs.)

IT 130753-29-6P 139528-27-1P 139528-28-2P 139528-29-3P 139528-30-6P 139528-31-7P 139528-32-8P 139528-33-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reduction by lithium aluminum hydride)
IT 139528-60-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 130753-27-4P 139528-26-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and regioselective substitution reactions of)
IT **2226-23-5P** 16256-83-0P 130563-29-0P 130563-30-3P
130563-31-4P 130753-24-1P 130753-28-5P 139528-34-0P 139528-35-1P
139528-36-2P 139528-37-3P 139528-38-4P 139528-39-5P 139528-40-8P
139528-41-9P 139528-42-0P 139528-43-1P 139528-44-2P 139528-45-3P
139528-46-4P 139528-47-5P 139528-48-6P 139528-49-7P 139528-50-0P
139528-51-1P 139528-52-2P 139528-53-3P 139528-54-4P 139528-55-5P
139528-56-6P 139528-57-7P 139528-58-8P 139528-59-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 524-38-9, N-Hydroxyphthalimide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with amino alcs.)
IT 85-41-6, 1H-Isoindole-1,3(2H)-dione
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ephedrine and pseudoephedrine derivs.)
IT 107-03-9, 1-Propanethiol 507-09-5, Thioacetic acid, reactions 829-85-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylephedrine)
IT 90-82-4 299-42-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective substitution by chlorodimethylacetamide)
IT 135711-20-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(sequential regioselective mesylation and imination by butylamine)
IT 552-79-4 48141-64-6 139627-69-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(sequential regioselective mesylation, azidation and reduction of)
IT 7005-47-2 64584-88-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective reactions of)
IT **2226-23-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2226-23-5 HCAPLUS
CN Ethanethioic acid, S-[2-(dimethylamino)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d all hitstr tot l38

L38 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2004:759870 HCAPLUS

ED Entered STN: 17 Sep 2004
TI Preparation of 2-aminoethanethiol compounds as efficient catalysts for asymmetric addition reaction
IN **Yang, Teng-Kuei**; Tseng, Shi-Liang; **Liu, To**; **Chen, Nan-Kuang**
PA Taiwan
SO U.S. Pat. Appl. Publ., 15 pp., Cont.-in-part of U.S. Pat. Appl. 2003 153,781.
CODEN: USXXCO
DT Patent
LA English
IC ICM C07D211-18
ICS C07D207-46; C07C027-18
NCL 540609000; 546232000; 548571000; 548950000; 548968000; 568878000
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): **29**, 25
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004181057	A1	20040916	US 2004-807710	20040323 <--
	US 2003153781	A1	20030814	US 2002-39557	20020108 <--
PRAI	US 2002-39557	A2	20020108 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 20040181057	ICM	C07D211-18
	ICS	C07D207-46; C07C027-18
	NCL	540609000; 546232000; 548571000; 548950000; 548968000; 568878000

AB The present invention discloses aminothiol compds. having a general formula R3R4NCH(R1)CH(R2)SR5 (wherein R1-R4 = aryl, C1-9 alkyl; or R3, R4 and N form a three- to eight-membered heterocycle; R5 = H, C1-6 alkyl). Such compds. can perform as superior catalysts for the synthesis of chiral secondary alcs. by asym. addition reaction of organic metal compds. such organozinc compound and **aldehyde**. According to the present invention, the aminothiol compds. are needed only less than 0.02% based on main reactants to obtain enantioselectivity higher than 98% enantiomeric excess, whereby the asym. reactions can become very economic. Thus, cycloalkylation of (2R,3S)-3-amino-4-methylpentan-2-ol by 1,4-dibromobutane in the presence of Na2CO3 in MeCN under refluxing for 12 h gave (2R,3S)-4-methyl-3-(1-pyrrolidinyl)pentan-2-ol which was treated with MeSO2Cl and Et3N in CH2Cl2 for 2 h at 0° for 2 h, concentrated, and reacted with thioacetic acid in benzene at room temperature for 12 h to give 20% (2R,3S)-4-methyl-3-(1-pyrrolidinyl)-2-thioacetylpentane (I) and 40% (3R,4S)-2-methyl-4-(1-pyrrolidinyl)-3-thioacetylpentane (II). I or II was reduced by LiAlH4 in Et2O at 0° for 1 h to give (2R,3S)-4-methyl-3-(1-pyrrolidinyl)pentane-2-thiol or (3R,4S)-2-methyl-4-(1-pyrrolidinyl)pentane-3-thiol (III) in 80% yield. Asym. addition reaction of benzaldehyde with Et2Zn in toluene in the presence of 0.05 mequiv. (equivalence concentration) III at -20° for 12 h gave (R)-2-phenylpropanol (99.6% ee). Chiral (R)-1-phenyl-2-alken-1-ols were also prepared from butylacetylene and hexylacetylene by monohydroboration of alkynes with BH3.SMe2 and transmetalation of boron to **zinc** with diethylzinc and asym. addition reaction with benzaldehyde or derivs. using the aminothiol catalysts.

ST **aldehyde** organometallic compd asym addn reaction; chiral secondary alc prepn; aminoethanethiol prepn asym addn reaction catalyst; methylpyrrolidinylpentanethiol prepn asym addn reaction catalyst; organozinc compd **aldehyde** asym addn reaction

IT Alcohols
RL: SPN (Synthetic preparation); PREP (Preparation)
(alkenols, 1-aryl-2-alkenols; preparation of 2-aminoethanethiol compds. as

catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

IT Thiols (organic)
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(amino; preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

IT Asymmetric synthesis and induction
(preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

IT **Aldehydes**
Organometallic compounds
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

IT Alcohols
RL: SPN (Synthetic preparation); PREP (Preparation)
(secondary, chiral; preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

IT **Addition reaction**
Addition reaction catalysts
(stereoselective; preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

IT Amines
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(thiol; preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

IT 160011-80-3P 571148-35-1P 757242-87-8P 757242-90-3P 757243-14-4P 757243-19-9P 757243-33-7P 757243-42-8P 757243-47-3P 757243-55-3P 757243-56-4P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(catalyst; preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

IT **160011-79-0P** 160167-27-1P 177320-30-8P 325781-90-6P **571148-36-2P** **571148-37-3P** 757242-70-9P **757242-81-2P** **757242-84-5P** 757242-94-7P **757243-04-2P** **757243-08-6P** 757243-26-8P 757243-36-0P **757243-39-3P** **757243-46-2P** **757243-54-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

IT 89-98-5, 2-Chlorobenzaldehyde 100-52-7, Benzaldehyde 110-52-1, 1,4-Dibromobutane 123-11-5, 4-Methoxybenzaldehyde 557-20-0, Diethylzinc 629-05-0, Hexylacetylene 693-02-7, Butylacetylene 7239-41-0, Bis(4-bromobutyl) ether 13292-87-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

IT 757243-45-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

IT 1565-74-8P, (R)-1-Phenylpropanol 757243-57-5P 757243-58-6P 757243-59-7P 757243-60-0P 757243-61-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

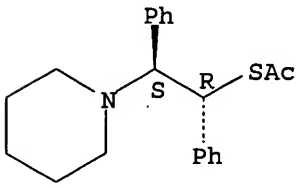
IT 111-24-0, 1,5-Dibromopentane 23190-16-1, (1R,2S)-2-Amino-1,2-diphenylethanol 111061-16-6 111138-89-7 215929-23-0 757242-98-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

IT **160011-79-0P 571148-36-2P 571148-37-3P**
757242-81-2P 757242-84-5P 757243-04-2P
757243-08-6P 757243-39-3P 757243-46-2P
757243-54-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of 2-aminoethanethiol compds. as catalysts for asym. addition reaction of organic metal compound with **aldehydes**)

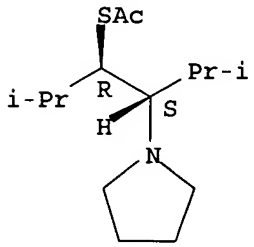
RN 160011-79-0 HCAPLUS
CN Ethanethioic acid, S-[1,2-diphenyl-2-(1-piperidinyl)ethyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



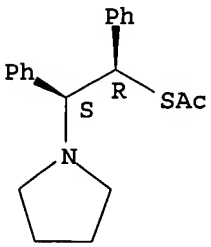
RN 571148-36-2 HCAPLUS
CN Ethanethioic acid, S-[(1R,2S)-3-methyl-1-(1-methylethyl)-2-(1-pyrrolidinyl)butyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



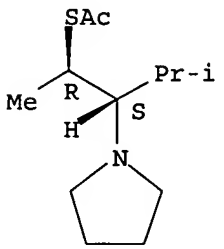
RN 571148-37-3 HCAPLUS
CN Ethanethioic acid, S-[(1R,2S)-1,2-diphenyl-2-(1-pyrrolidinyl)ethyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



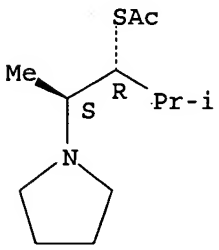
RN 757242-81-2 HCAPLUS
CN Ethanethioic acid, S-[(1R,2S)-1,3-dimethyl-2-(1-pyrrolidinyl)butyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



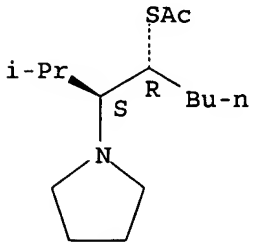
RN 757242-84-5 HCAPLUS
CN Ethanethioic acid, S-[(1R,2S)-1-(1-methylethyl)-2-(1-pyrrolidinyl)propyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+)..



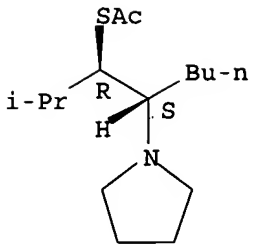
RN 757243-04-2 HCAPLUS
CN Ethanethioic acid, S-[(1R)-1-[(1S)-2-methyl-1-(1-pyrrolidinyl)propyl]pentyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



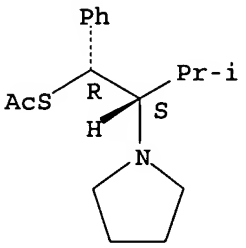
RN 757243-08-6 HCAPLUS
CN Ethanethioic acid, S-[(1R,2S)-1-(1-methylethyl)-2-(1-pyrrolidinyl)hexyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



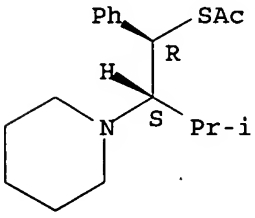
RN 757243-39-3 HCAPLUS
CN Ethanethioic acid, S-[(1R,2S)-3-methyl-1-phenyl-2-(1-pyrrolidinyl)butyl] ester (9CI). (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



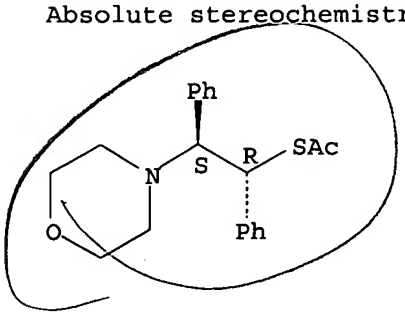
RN 757243-46-2 HCAPLUS
CN Ethanethioic acid, S-[(1R,2S)-3-methyl-1-phenyl-2-(1-piperidinyl)butyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 757243-54-2 HCAPLUS
CN Ethanethioic acid, S-[(1R,2S)-2-(4-morpholinyl)-1,2-diphenylethyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L38 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:633325 HCAPLUS

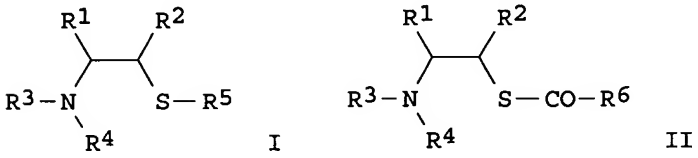
DN 139:149522
ED Entered STN: 15 Aug 2003
TI Aminothiol compounds and acylated derivatives thereof
IN **Yang, Teng-Kuei; Chen, Nan-Kuang; Liu, To**
PA Taiwan
SO U.S. Pat. Appl. Publ., 5 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM C07C239-06
ICS C07D265-30
NCL 558250000; 564340000; 544158000
CC 27-10 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): **29**
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI US 2003153781	A1	20030814	US 2002-39557	20020108	<--
US 2004049033	A1	20040311	US 2003-650020	20030826	<--
US 2004181057	A1	20040916	US 2004-807710	20040323	<--
PRAI US 2002-39557	A3	20020108	<--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
US 2003153781	ICM	C07C239-06	
	ICS	C07D265-30	
	NCL	558250000; 564340000; 544158000	
US 2004049033	ECLA	C07D295/08B1F; C07D295/08B1B	<--

OS MARPAT 139:149522
GI



I II

AB The present invention discloses aminothiol compds. and acylated derivs. I and II (R1, R2, R3, R4 = C1-9-alkyl or NR3R4 = 3-8-membered heterocycle, R5 and R6 = H, C1-6-alkyl) are substitutable **ligands.** For example, 1,2-diphenyl-2-pyrrolidinylethanethiol was prepared by the reaction of (1R,2S)-1,2-diphenyl-2-aminoethanol with 1,4-dibromobutane, followed by reaction of MeSO3Cl and reduction by LiAlH4. Such compds. can perform as superior catalysts in asym. addition reactions of organic **Zn** and **aldehyde.** According to the present invention, the compds. needed only <0.02% of main reactants to obtain enantioselectivity >99% enantiomeric excess, whereby the asym. reactions can become very economic.

ST aminothiol prepn asym addn catalyst
IT **Aldehydes**, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aminothiols as asym. addition catalyst with organozinc complexes with **aldehydes**)
IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of aminothiols as asym. addition catalyst with organozinc complexes with **aldehydes** in preparation of alcs.)
IT **Addition reaction catalysts**
(stereoselective; preparation of aminothiol **ligands** as)
IT **571148-37-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactant for preparation of aminothiols as asym. addition catalyst
with organozinc complexes with **aldehydes**)

IT 160011-80-3P 571148-35-1P **571148-36-2P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as asym. addition catalyst with organozinc complexes with **aldehydes**)

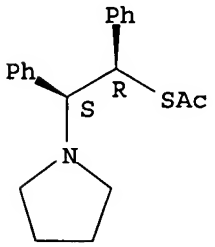
IT **7440-32-6D, Titanium**, organo **7440-50-8D, Copper**, organo **7440-66-6D, Zinc**, organo
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aminothiols as asym. addition catalyst with organozinc complexes with **aldehydes**)

IT 110-52-1, 1,4-Dibromobutane 23190-16-1, (1R,2S)-1,2-Diphenyl-2-aminoethanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for preparation of aminothiols as asym. addition catalyst with organozinc complexes with **aldehydes**)

IT **571148-37-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactant for preparation of aminothiols as asym. addition catalyst
with organozinc complexes with **aldehydes**)

RN 571148-37-3 HCAPLUS
CN Ethanethioic acid, S-[(1R,2S)-1,2-diphenyl-2-(1-pyrrolidinyl)ethyl] ester (9CI) (CA INDEX NAME)

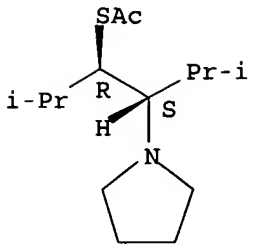
Absolute stereochemistry. Rotation (-).



IT **571148-36-2P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as asym. addition catalyst with organozinc complexes with **aldehydes**)

RN 571148-36-2 HCAPLUS
CN Ethanethioic acid, S-[(1R,2S)-3-methyl-1-(1-methylethyl)-2-(1-pyrrolidinyl)butyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT **7440-32-6D, Titanium**, organo **7440-50-8D, Copper**, organo **7440-66-6D, Zinc**, organo
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aminothiols as asym. addition catalyst with organozinc complexes with **aldehydes**)
RN 7440-32-6 HCAPLUS
CN Titanium (8CI, 9CI) (CA INDEX NAME)

Ti

RN 7440-50-8 HCAPLUS
CN Copper (7CI, 8CI, 9CI) (CA INDEX NAME)

Cu

RN 7440-66-6 HCAPLUS
CN Zinc (7CI, 8CI, 9CI) (CA INDEX NAME)

Zn

=> => fil uspatall
FILE 'USPATFULL' ENTERED AT 15:32:02 ON 13 OCT 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 15:32:02 ON 13 OCT 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

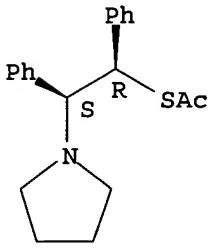
=> d l42 bib abs hitstr tot

L42 ANSWER 1 OF 2 USPATFULL on STN
AN 2004:64514 USPATFULL
TI Acylated aminothiol compound
IN Yang, Teng-Kuei, Taichung, TAIWAN, PROVINCE OF CHINA
Chen, Nan-Kuang, Taichung, TAIWAN, PROVINCE OF CHINA
Liu, To, Taichung, TAIWAN, PROVINCE OF CHINA
PI US 2004049033 A1 20040311
AI US 2003-650020 A1 20030826 (10)
RLI Division of Ser. No. US 2002-39557, filed on 8 Jan 2002, PENDING
DT Utility
FS APPLICATION
LREP CHARLES E. BAXLEY, ESQUIRE, Third Floor, 90 John Street,, New York, NY, 10038
CLMN Number of Claims: 8

ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 197
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The present invention discloses an acylated derivative of an aminothiol compound having a general formula II wherein R.sup.1-R.sup.4 and R.sup.6 are substitutable ligands. Such compounds can perform as superior catalysts in asymmetric addition reactions of organic zinc and aldehyde. According to the present invention, only less than 0.02% of the acylated derivative is needed to obtain high enantioselectivity over 99% enantiomeric excess. ##STR1##

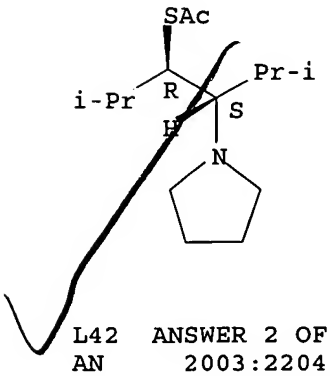
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **571148-37-3P**
(preparation and reactant for preparation of aminothiols as asym. addition catalyst
with organozinc complexes with aldehydes)
RN 571148-37-3 USPATFULL
CN Ethanethioic acid, S-[(1R,2S)-1,2-diphenyl-2-(1-pyrrolidinyl)ethyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **571148-36-2P**
(preparation as asym. addition catalyst with organozinc complexes with aldehydes)
RN 571148-36-2 USPATFULL
CN Ethanethioic acid, S-[(1R,2S)-3-methyl-1-(1-methylethyl)-2-(1-pyrrolidinyl)butyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

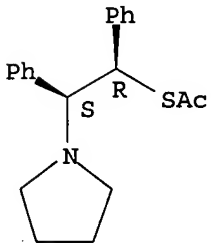


L42 ANSWER 2 OF 2 USPATFULL on STN
AN 2003:220490 USPATFULL
TI AMINOTHIOL COMPOUNDS AND ACYLATED DERIVATIVES THEREOF
IN Yang, Teng-Kuei, Taichung, TAIWAN, PROVINCE OF CHINA
Chen, Nan-Kuang, Taichung, TAIWAN, PROVINCE OF CHINA
Liu, To, Taichung, TAIWAN, PROVINCE OF CHINA
PI US 2003153781 A1 20030814
AI US 2002-39557 A1 20020108 (10)

DT Utility
FS APPLICATION
LREP Hart, Baxley, Daniels & Holton, Fifth Floor, 59 John Street, New York, NY, 10038
CLMN Number of Claims: 19
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 264
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The present invention discloses aminothiol compounds and acylated derivatives thereof, which respectively have general formula I and formula II wherein R.sup.1-R.sup.6 are substitutable ligands. Such compounds can perform as superior catalysts in asymmetric addition reactions of organic zinc and aldehyde. According to the present invention, the compounds is needed only less than 0.02% of main reactants to obtain enantioselectivity higher than 99% enantiomeric excess, whereby the asymmetric reactions can become very economic. ##STR1##

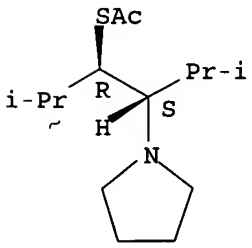
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **571148-37-3P**
(preparation and reactant for preparation of aminothiols as asym. addition catalyst
with organozinc complexes with aldehydes)
RN 571148-37-3 USPATFULL
CN Ethanethioic acid, S-[(1R,2S)-1,2-diphenyl-2-(1-pyrrolidinyl)ethyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **571148-36-2P**
(preparation as asym. addition catalyst with organozinc complexes with aldehydes)
RN 571148-36-2 USPATFULL
CN Ethanethioic acid, S-[(1R,2S)-3-methyl-1-(1-methylethyl)-2-(1-pyrrolidinyl)butyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



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=> d his

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L1             2 S (US2002-039557# OR US2003-650020#)/AP,PRN
               E YANG T/AU
L2           187 S E3,E20,E21
               E YANG TENG/AU
L3            49 S E3,E10
L4             3 S E13
               E CHEN N/AU
L5            99 S E3,E14
               E CHEN NAN/AU
L6           131 S E3,E15
               E LIU T/AU
L7           822 S E3-E37
               E LIU TO/AU
L8             2 S E3
L9           483 S LIU TO?/AU
L10            2 S L1 AND L2-L9
               SEL RN

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L11           53 S E1-E53
L12           11 S L11 AND (N AND S AND O)/ELS
L13               STR
L14            1 S L13 CSS SAM
L15           25 S L13 CSS FUL
               SAV L15 SHIAO650/A
L16           10 S L11 AND L15
L17            1 S L12 NOT L16
L18           15 S L15 NOT L16
L19           13 S L18 NOT (C19H21NOS OR C25H25NOS)
L20            2 S L18 NOT L19
L21           23 S L16,L19

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L22            3 S L21
               SEL AN
               EDIT E54-E56 /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 15:23:10 ON 13 OCT 2004
L23            5 S E54-E56

     FILE 'HCAOLD' ENTERED AT 15:23:42 ON 13 OCT 2004

     FILE 'HCAPLUS' ENTERED AT 15:24:43 ON 13 OCT 2004
L24            4 S L23 NOT ASINGER ?/AU
L25           12 S L21
L26            2 S L25 AND L1-L10
L27           14 S L24-L26
               E ADDITION REACTION/CT
L28            8 S L27 AND (E3+OLD,NT,PFT,RT OR E46+OLD,NT,PFT,RT OR E58+OLD,NT,
L29            7 S L27 AND (ALDEHYDE OR KETONE)
L30            0 S L27 AND CARBONYL
L31            4 S L27 AND LIGAND

     FILE 'REGISTRY' ENTERED AT 15:27:43 ON 13 OCT 2004
L32            3 S (ZINC OR COPPER OR TITANIUM)/CN

     FILE 'HCAPLUS' ENTERED AT 15:28:04 ON 13 OCT 2004
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L33           1 S L27 AND L32
L34           4 S L27 AND (ZN OR ZINC OR CU OR COPPER OR TI OR TITAN?)
L35           0 S L27 AND ?METAL?(L)?COMPLEX?
L36          14 S L27-L31,L33-L35
L37          14 S L36 AND (PD<=20020108 OR PRD<=20020108 OR AD<=20020108)
L38           2 S L37 AND ORGANOMETAL?/SC,SX
L39          12 S L37 NOT L38
L40           4 S L39 AND L24
L41           8 S L39 NOT L40

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     FILE 'HCAPLUS' ENTERED AT 15:30:58 ON 13 OCT 2004

     FILE 'USPATFULL, USPAT2' ENTERED AT 15:31:43 ON 13 OCT 2004
L42           2 S L21

     FILE 'USPATFULL, USPAT2' ENTERED AT 15:32:02 ON 13 OCT 2004

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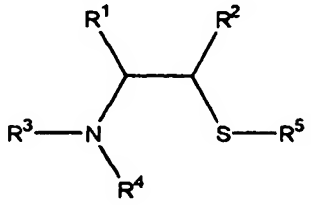
Amendments to the Claims:

This listing of claims will replace all prior versions, and listings, of claims in the application:

Listing of Claims:

Claim 1 (currently amended): An aminothiol compounds, having a general formula I,



I

wherein R^1-R^5 are substitutable ligands; and

R^1 is aryl ;

R^2 is aryl or alkyl of C1-C9;

R^3 is alkyl of C1-C9;

R^4 is alkyl of C1-C9; or

R^3, R^4 and N form a ~~three-to-eight-membered~~ five-membered heterocycle; and

R^5 is ~~H or alkyl of C1-C6~~.

Claims 2-14 (previously canceled)

Claim 15 (currently canceled)

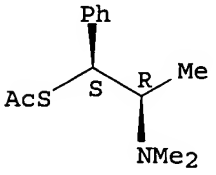
Claims 16-19 (previously canceled)

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1965:8904 CAPLUS
DOCUMENT NUMBER: 62:8904
ORIGINAL REFERENCE NO.: 62:1588a-c
TITLE: Phenylmercaptoalkylamines. III. Hofmann degradation of 1-phenyl-2-dimethylaminopropanethiol quaternary salts
AUTHOR(S): Nishimura, Haruki; Takamatsu, Hideji
CORPORATE SOURCE: Dainippon Pharm. Co., Ltd., Osaka, Japan
SOURCE: Yakugaku Zasshi (1964), 84(9), 811-17
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB Na2S2O3 and L-(+)-threo-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl, followed by hydrolysis, gave (+)-1-phenyl-2-dimethylaminopropanethiol (I), which was then converted into the methiodide and treated with NaOH to form (+)-1,2-epithiopropylbenzene (II), b10 100°, which was polymerized to give a polymer, m. 255-6°. Treatment of D-(+)-erythro-1,2-epoxypropylbenzene with KSCN gave L-(-)-erythro-1,2-epithiopropylbenzene, b7 92-3°, [α]20D -21.4° (c 2.21, MeOH), which was found to be the antipode of II. II belongs to the D-(+)-erythro series and I, to the L-(+)-threo series. The (-)-amino thiol, similarly derived from L-(-)-erythro-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl, was found to belong to the L-(-)-erythro series and that D-(+)-threo-1,2-epithiopropylbenzene (III) is derived from it. The steric configuration of II and III was also determined from their N.M.R. spectra. Hofmann degradation of the quaternary salt of 1-phenyl-2-dimethylaminoethanethiol also gave the same result. II and III underwent desulfurization by heating to give trans-β-methylstyrene.

IT **1210-30-6**, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, acetate (ester), L(-)-erythro-
(preparation of)
RN 1210-30-6 CAPLUS
CN Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester, erythro- (8CI) (CA INDEX NAME)

Relative stereochemistry.



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

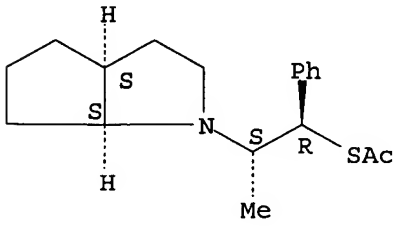
ACCESSION NUMBER: 1999:497835 CAPLUS
DOCUMENT NUMBER: 131:350834
TITLE: Utilization of industrial waste materials. Part 14. Synthesis of β-amino alcohols and thiols with a 2-azabicyclo[3.3.0]octane backbone and their application in enantioselective catalysis
AUTHOR(S): Kossenjans, Michael; Soeberdt, Michael; Wallbaum, Sabine; Harms, Klaus; Martens, Jurgen; Aurich, Hans Gunter
CORPORATE SOURCE: Fachbereich Chemie, Universitat Oldenburg, Oldenburg, D-26129, Germany
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (16), 2353-2365
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:350834

AB New, chiral β-tert-amino tert-alcs. were synthesized from an enantiomerically pure sec-amine via glycine, alanine and phenylglycine derivs. Grignard addns. to these esters provided rigid amino alcs. in fair yields. The absolute configurations of the stereogenic centers, which arose during the alkylation step, were assigned by an independent route leading to some of the optical antipodes. The target compds. were derivs. of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol. Condensation of enantiomerically pure β-amino alcs. with a γ-keto ester afforded N,O-acetals which were subsequently reduced to the β-tert-amino alcs. X-Ray anal. of one compound was performed to verify the stereochem. observed by chemical correlation. The nucleophilic ring opening of enantiomerically pure styrene oxide by an amine resulted in the formation of regioisomeric amino alcs. Amino thiol derivs. were also prepared Reduction of these compds. to thiols and subsequent oxidation afforded amino disulfides. Finally, the bicyclic β-amino alcs. and thiols were used as chiral ligands in the enantioselective addition of diethylzinc to benzaldehyde and ee values up to 96% were found.

IT **250371-17-6P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

RN 250371-17-6 CAPLUS
CN Ethanethioic acid, S-[(1R,2S)-2-[(3aS,6aS)-hexahydrocyclopenta[b]pyrrol-1(2H)-yl]-1-phenylpropyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

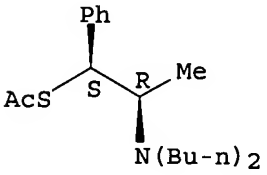
ACCESSION NUMBER: 1998:569540 CAPLUS
DOCUMENT NUMBER: 129:289723
TITLE: Zirconocene-Zinc Transmetalation and in Situ Catalytic Asymmetric Addition to Aldehydes
AUTHOR(S): Wipf, Peter; Ribe, Seth
CORPORATE SOURCE: Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of Organic Chemistry (1998), 63(19), 6454-6455
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The in situ hydrozirconation of alkynes, trans-metalation to dimethylzinc and chiral amino thiol-catalyzed addition to aldehydes provided an efficient protocol for the asym. preparation of (E)-allylic alcs. For example, the hydrozirconation of 1-hexyne, followed by transmetalation via addition of dimethylzinc and sequential addition of the resulting (alkenyl)methylzinc intermediate to benzaldehyde gave [S-(E)]-1-phenyl-2-hepten-1-ol [i.e., [S-(E)]-α-(1-hexenyl)benzenemethanol] in 90% and in 83% enantiomeric excess. The last step in the sequence was catalyzed in the presence of (R)-2-[1-(dimethylamino)propyl]benzenethiol as ligand.

IT **185606-94-4**
RL: CAT (Catalyst use); USES (Uses)
(preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to aldehydes)

RN 185606-94-4 CAPLUS
CN Ethanethioic acid, S-[(1S,2R)-2-(dibutylamino)-1-phenylpropyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

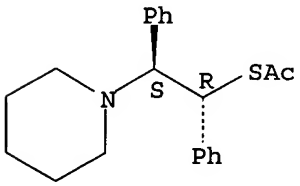
ACCESSION NUMBER: 1997:39785 CAPLUS
DOCUMENT NUMBER: 126:131036
TITLE: Chiral β-amino thiol catalysts for the enantioselective addition of diethylzinc to aldehydes
AUTHOR(S): Kang, Jahyo; Kim, Jeong Whan; Lee, Jun Won; Kim, Dong Soo; Kim, Joo In
CORPORATE SOURCE: Dep. Chem., Sogang Univ., Seoul, 121-742, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (1996), 17(12), 1135-1142
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Reaction of diethylzinc with α-branched aldehydes in the presence of a catalytic amount (5 mol %) of various β-amino thiols in toluene or ether provided the corresponding secondary alcs. in outstanding ee. Detailed preparative procedure for the β-amino thiols are presented.

IT **160011-79-0P 166031-45-4P 166031-48-7P 186314-11-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective addition of diethylzinc to aldehydes using chiral β-amino thiol catalysts)

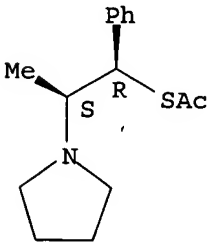
RN 160011-79-0 CAPLUS
CN Ethanethioic acid, S-[(1R,2S)-1,2-diphenyl-2-(1-piperidinyl)ethyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



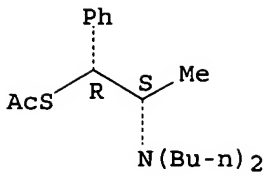
RN 166031-45-4 CAPLUS
CN Ethanethioic acid, S-[1-phenyl-2-(1-pyrrolidinyl)propyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



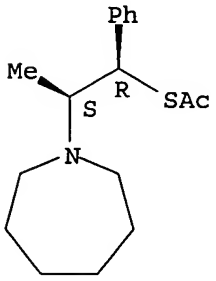
RN 166031-48-7 CAPLUS
CN Ethanethioic acid, S-[2-(dibutylamino)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



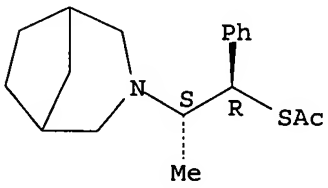
RN 186314-11-4 CAPLUS
CN Ethanethioic acid, S-[2-(hexahydro-1H-azepin-1-yl)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **186314-19-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective addition of diethylzinc to aldehydes using chiral β-amino thiol catalysts)
RN 186314-19-2 CAPLUS
CN Ethanethioic acid, S-[2-(3-azabicyclo[3.2.1]oct-3-yl)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

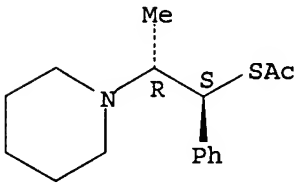
ACCESSION NUMBER: 1996:729946 CAPLUS
DOCUMENT NUMBER: 126:103872
TITLE: New chiral catalysts for the highly enantioselective addition of diethylzinc to aldehydes
AUTHOR(S): Jin, Myung-Jong; Ahn, Sum-Jin; Lee, Kyoung-Soo
CORPORATE SOURCE: Dep. Chemical Engineering, Inha Univ., Inchon, 402-751, S. Korea
SOURCE: Tetrahedron Letters (1996), 37(48), 8767-8770
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Optically active amino thioacetate derivs. of (+)-norephedrine were found to act as effective catalysts for enantioselective addition of diethylzinc to aldehydes. This reaction provided optically active secondary alcs. with e.e. of up to >99%.

IT **185606-97-7**
RL: CAT (Catalyst use); USES (Uses)
(chiral catalysts for enantioselective addition of diethylzinc to aldehydes)

RN 185606-97-7 CAPLUS
CN Ethanethioic acid, S-[1-phenyl-2-(1-piperidinyl)propyl] ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

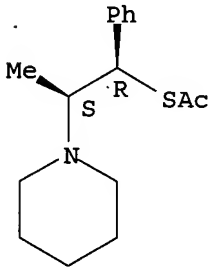
ACCESSION NUMBER: 1995:86424 CAPLUS
DOCUMENT NUMBER: 123:142957
TITLE: Enantioselective addition of diethylzinc to α-branched aldehydes
AUTHOR(S): Kang, Jahyo; Lee, Jun Won; Kim, Joo In
CORPORATE SOURCE: Department of Chemistry, Sogang University, Seoul, 121-742, S. Korea
SOURCE: Journal of the Chemical Society, Chemical Communications (1994), (17), 2009-10
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Reaction of diethylzinc with α-branched aldehydes in the presence of a catalytic amount of (1R,2S)-(-)-1-phenyl-2-piperidinopropane-1-thiol provided the corresponding secondary alcs. in almost 100% enantiomeric excess.

IT **166031-44-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthetic intermediate; in conversion to ligand catalyst for enantioselective addition of diethylzinc to α-branched aldehydes)

RN 166031-44-3 CAPLUS
CN Ethanethioic acid, S-[1-phenyl-2-(1-piperidinyl)propyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

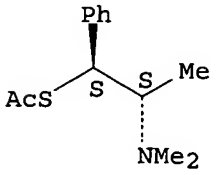
ACCESSION NUMBER: 1994:680925 CAPLUS
DOCUMENT NUMBER: 121:280925
TITLE: Nucleophilic substitutions using O-alkyl-N,N'-dialkylisoureas. Applications to ephedrines
AUTHOR(S): Poelert, Martin A.; Hulshof, L. A.; Kellogg, Richard M.
CORPORATE SOURCE: Dep. Organic Chemi., Univ. Groningen, Groningen, 9747 AG, Neth.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1994), 113(7-8), 365-8
CODEN: RTCPA3; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:280925

AB Dialkylcarbodiimides in the presence of a CuI catalyst react cleanly with the hydroxyl group of N-methylated (1R,2S)-ephedrine and (1S,2S)-pseudoephedrine. These adducts react with nucleophiles like alkyl and aryl thiols as well as thioic acids and phthalimide to form the substitution products with overall retention of configuration. It is postulated that intramol. participation of the amino group via an SN2 reaction leads to aziridinium salts, which are subsequently opened by the nucleophiles via a second SN2 reaction. This synthetic approach is also useful for the inversion of simple secondary alcs.; on treatment with dicyclohexylcarbodiimide followed by benzothioic acid and treatment with LiAlH4, menthol was converted in good yield to neomenthane thiol.

IT **2226-22-4P 2226-23-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(nucleophilic substitutions using alkyldialkylisoureas, applications to ephedrines)

RN 2226-22-4 CAPLUS
CN Ethanethioic acid, S-[2-(dimethylamino)-1-phenylpropyl] ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 2226-23-5 CAPLUS
CN Ethanethioic acid, S-[2-(dimethylamino)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.